Full wwPDB X-ray Structure Validation Report (i)

Jun 10, 2024 – 05:14 PM EDT

PDB ID	:	8W0Z
Title	:	Human LCAD complexed with Lauric Acid
Authors	:	Xia, C.; Kim, J.J.P.
Deposited on	:	2024-02-14
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

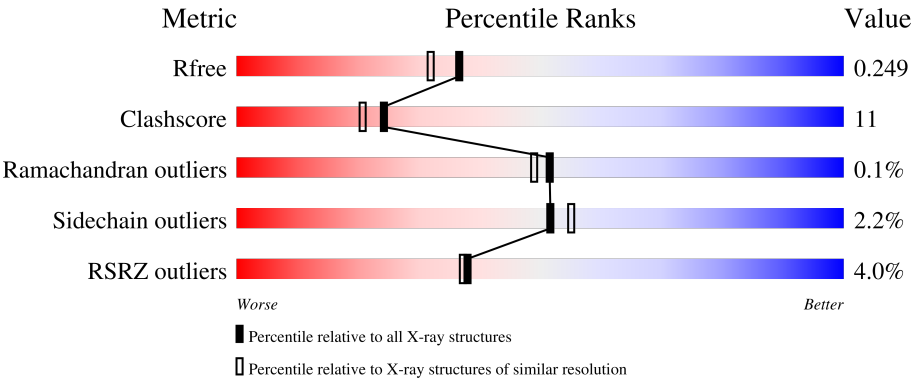
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	400	2% 76% 22%
1	B	400	4% 74% 24%
1	C	400	2% 80% 17%
1	D	400	7% 72% 26%
1	E	400	2% 80% 18%

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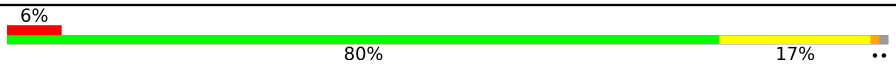
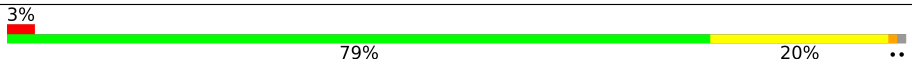
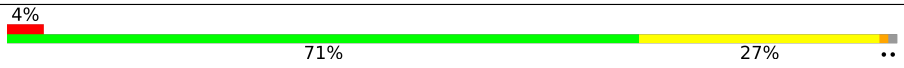
Mol	Chain	Length	Quality of chain
1	F	400	
1	G	400	
1	H	400	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DAO	A	502	-	-	-	X
3	DAO	B	502	-	-	-	X
3	DAO	C	502	-	-	-	X
3	DAO	D	502	-	-	-	X
3	DAO	E	502	-	-	-	X
3	DAO	F	502	-	-	-	X
3	DAO	G	502	-	-	-	X
3	DAO	H	502	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27170 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

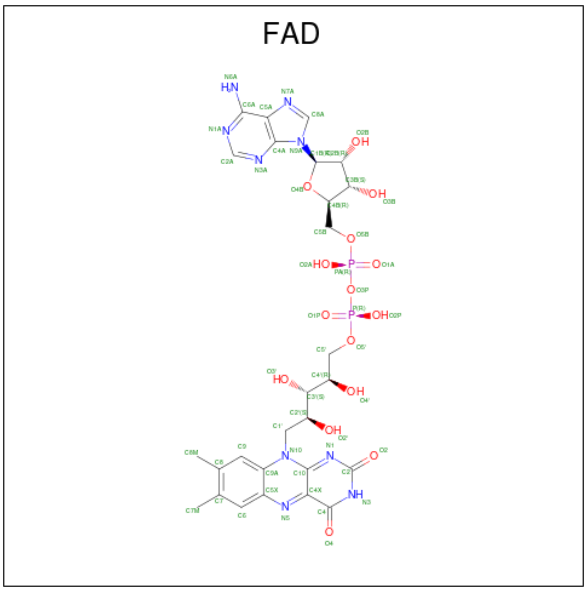
- Molecule 1 is a protein called Long-chain specific acyl-CoA dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3094	1972	535	571	16			
1	B	396	Total	C	N	O	S	0	0	0
			3102	1976	536	574	16			
1	C	395	Total	C	N	O	S	0	0	0
			3094	1972	535	571	16			
1	D	395	Total	C	N	O	S	0	0	0
			3094	1972	535	571	16			
1	E	395	Total	C	N	O	S	0	0	0
			3094	1972	535	571	16			
1	F	396	Total	C	N	O	S	0	0	0
			3102	1976	536	574	16			
1	G	396	Total	C	N	O	S	0	0	0
			3102	1976	536	574	16			
1	H	395	Total	C	N	O	S	0	0	0
			3094	1972	535	571	16			

There are 8 discrepancies between the modelled and reference sequences:

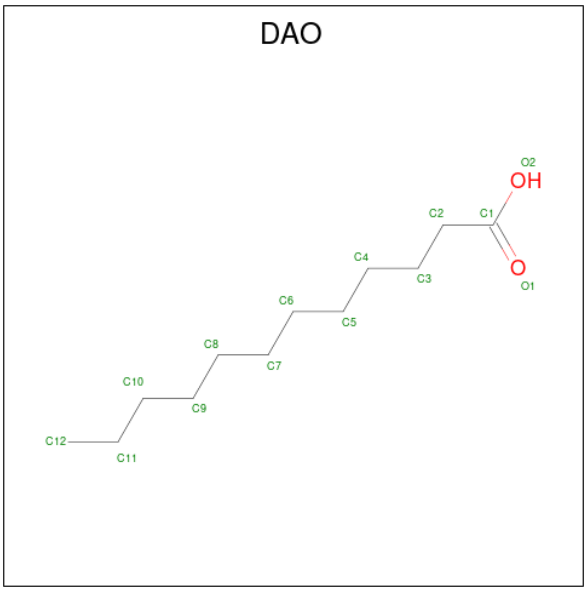
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLN	GLU	engineered mutation	UNP P28330
B	291	GLN	GLU	engineered mutation	UNP P28330
C	291	GLN	GLU	engineered mutation	UNP P28330
D	291	GLN	GLU	engineered mutation	UNP P28330
E	291	GLN	GLU	engineered mutation	UNP P28330
F	291	GLN	GLU	engineered mutation	UNP P28330
G	291	GLN	GLU	engineered mutation	UNP P28330
H	291	GLN	GLU	engineered mutation	UNP P28330

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	C	1	Total C O 14 12 2	0	0
3	D	1	Total C O 14 12 2	0	0
3	E	1	Total C O 14 12 2	0	0
3	F	1	Total C O 14 12 2	0	0
3	G	1	Total C O 14 12 2	0	0
3	H	1	Total C O 14 12 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	247	Total O 247 247	0	0
4	B	210	Total O 210 210	0	0
4	C	234	Total O 234 234	0	0
4	D	189	Total O 189 189	0	0

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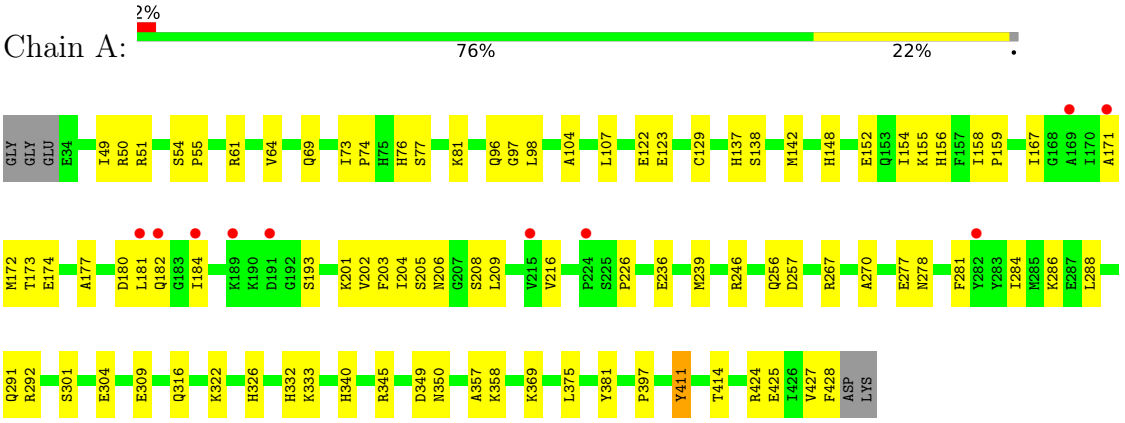
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	277	Total O 277 277	0	0
4	F	244	Total O 244 244	0	0
4	G	239	Total O 239 239	0	0
4	H	218	Total O 218 218	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

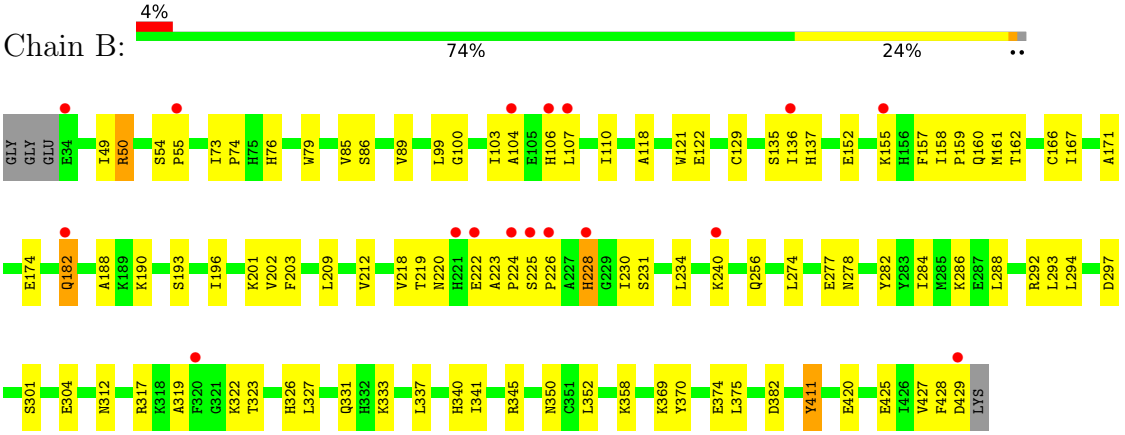
• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain A:



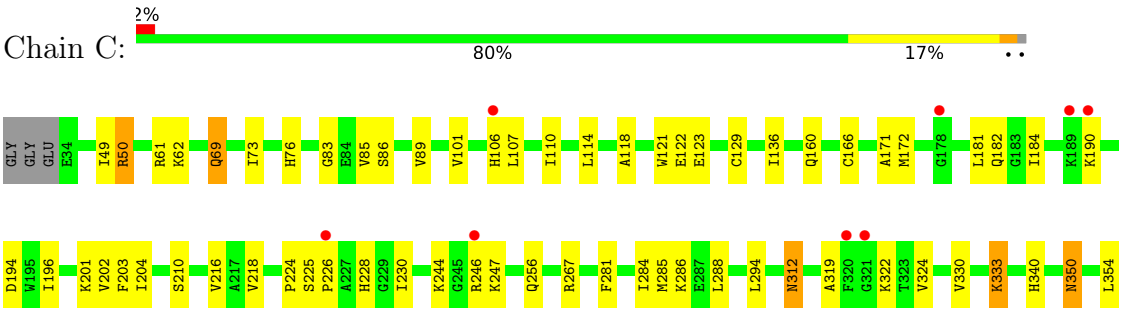
• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

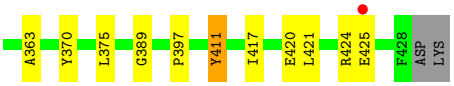
Chain B:



• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

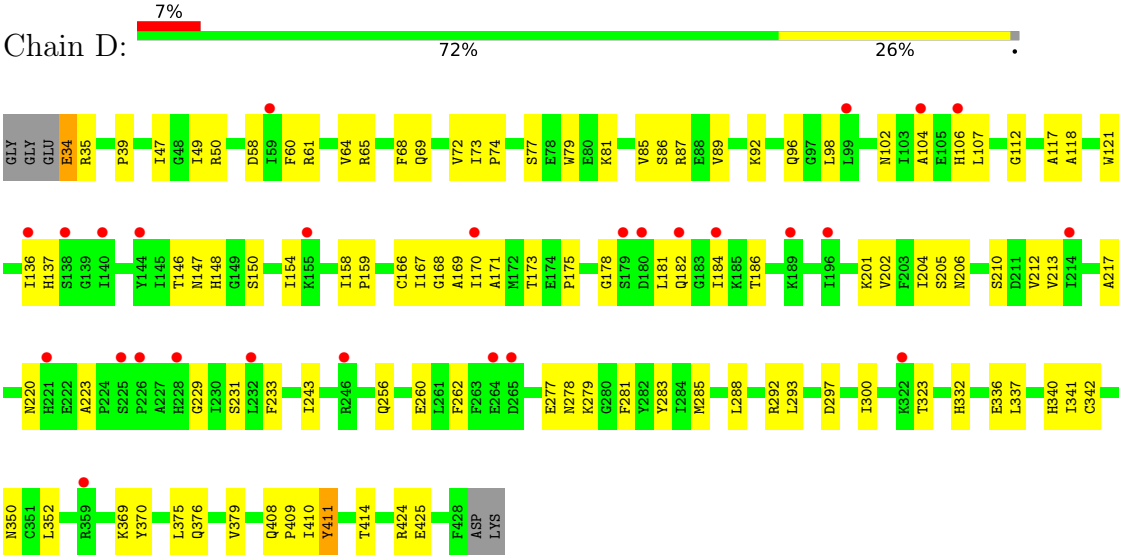
Chain C:





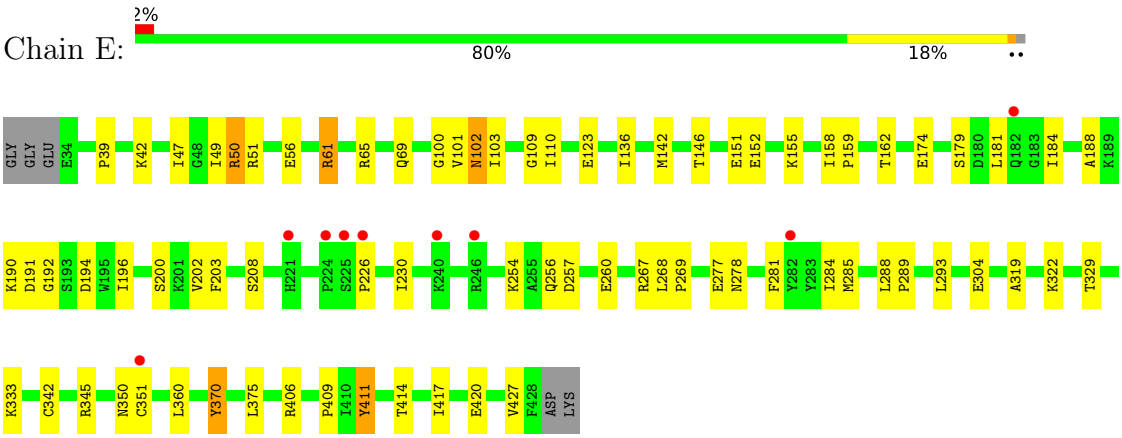
• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain D:



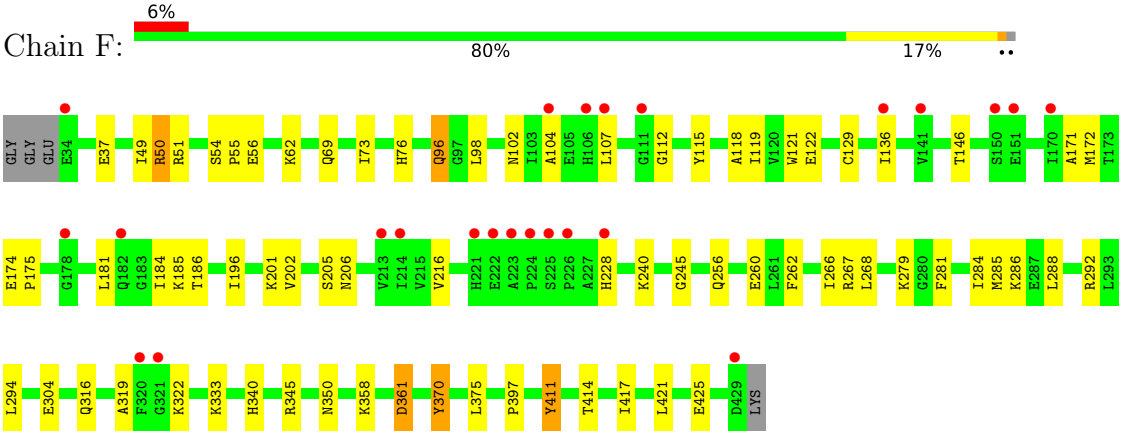
• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain E:



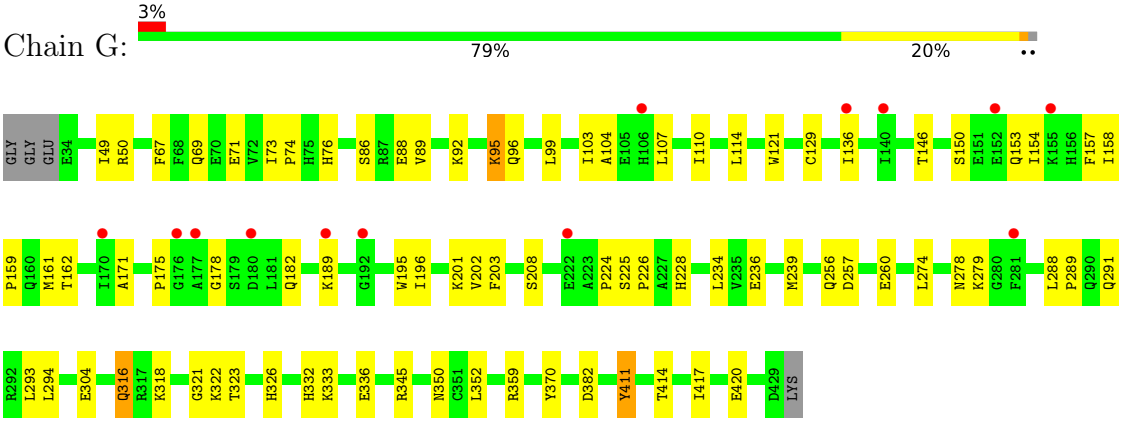
• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain F:



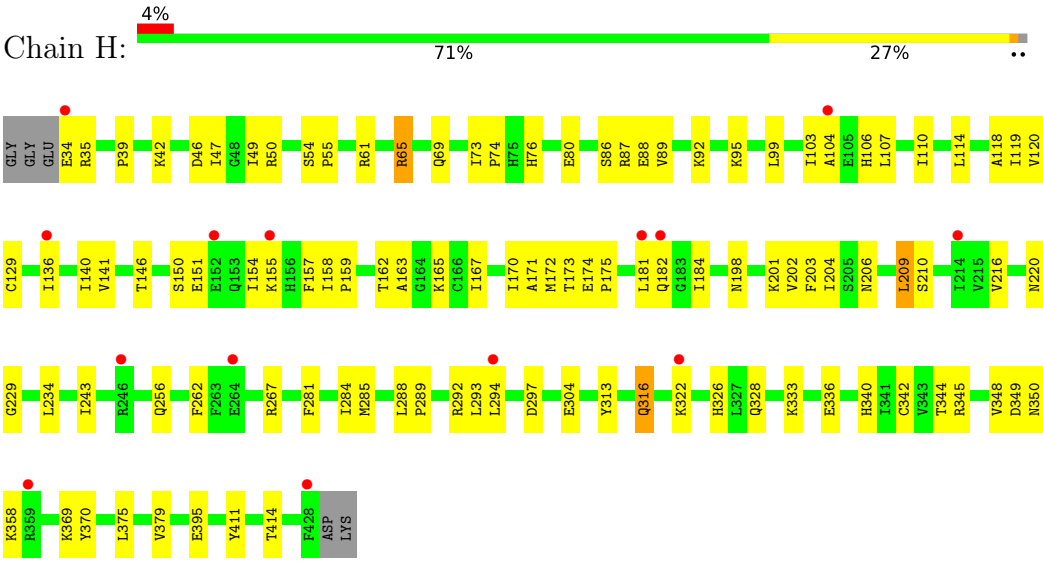
• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain G:



• Molecule 1: Long-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.29Å 94.84Å 119.16Å 89.24° 74.88° 88.35°	Depositor
Resolution (Å)	30.12 – 2.00 30.12 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.12-2.00) 94.5 (30.12-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.96Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.214 , 0.256 0.209 , 0.249	Depositor DCC
R_{free} test set	11840 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.106 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27170	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, DAO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/3163	0.56	0/4267
1	B	0.34	0/3171	0.57	0/4278
1	C	0.33	0/3163	0.57	0/4267
1	D	0.32	0/3163	0.54	0/4267
1	E	0.37	0/3163	0.59	0/4267
1	F	0.34	0/3171	0.59	0/4278
1	G	0.35	0/3171	0.58	0/4278
1	H	0.33	0/3163	0.56	0/4267
All	All	0.34	0/25328	0.57	0/34169

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3094	0	3073	76	0
1	B	3102	0	3077	73	0
1	C	3094	0	3073	69	0
1	D	3094	0	3073	76	0
1	E	3094	0	3073	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3102	0	3077	60	0
1	G	3102	0	3077	64	0
1	H	3094	0	3073	84	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
2	E	53	0	31	1	0
2	F	53	0	31	0	0
2	G	53	0	31	1	0
2	H	53	0	31	2	0
3	A	14	0	23	3	0
3	B	14	0	23	2	0
3	C	14	0	23	2	0
3	D	14	0	23	3	0
3	E	14	0	23	2	0
3	F	14	0	23	5	0
3	G	14	0	23	2	0
3	H	14	0	23	2	0
4	A	247	0	0	10	0
4	B	210	0	0	5	0
4	C	234	0	0	7	0
4	D	189	0	0	4	0
4	E	277	0	0	10	0
4	F	244	0	0	15	0
4	G	239	0	0	9	0
4	H	218	0	0	13	0
All	All	27170	0	25028	556	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (556) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.42	0.84
1:B:161:MET:HE1	1:B:212:VAL:HG11	1.56	0.84
1:D:171:ALA:HB1	1:D:201:LYS:HG3	1.60	0.83
1:E:427:VAL:HB	4:G:769:HOH:O	1.78	0.82
1:D:292:ARG:HG3	1:D:292:ARG:HH11	1.44	0.81
1:A:286:LYS:HE2	4:A:614:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:SER:O	1:A:81:LYS:HD3	1.81	0.79
1:A:182:GLN:HG3	1:A:226:PRO:HG2	1.65	0.78
1:E:304:GLU:OE2	1:E:345:ARG:HD2	1.82	0.78
1:C:417:ILE:O	1:C:421:LEU:HD23	1.86	0.74
1:H:182:GLN:HG3	1:H:226:PRO:HG3	1.69	0.74
1:F:202:VAL:HB	4:F:730:HOH:O	1.89	0.72
1:F:286:LYS:HE2	1:F:286:LYS:HA	1.72	0.72
3:E:502:DAO:H92	4:E:755:HOH:O	1.89	0.71
1:F:96:GLN:HB3	1:F:98:LEU:HD13	1.73	0.71
1:B:333:LYS:HE2	1:B:382:ASP:HB3	1.73	0.71
1:C:181:LEU:O	1:C:184:ILE:HG12	1.91	0.70
1:C:160:GLN:HG2	1:C:166:CYS:HB2	1.73	0.70
1:B:157:PHE:HB3	1:B:161:MET:HE3	1.74	0.69
1:D:220:ASN:HB3	1:D:229:GLY:HA2	1.75	0.69
1:B:167:ILE:HD13	1:B:209:LEU:HD13	1.74	0.69
1:F:292:ARG:HG3	1:F:292:ARG:HH11	1.56	0.69
1:A:138:SER:HA	1:A:142:MET:HE2	1.75	0.68
1:H:181:LEU:HD23	1:H:181:LEU:H	1.58	0.68
1:C:201:LYS:HB3	1:C:204:ILE:HD11	1.74	0.68
1:A:425:GLU:HB2	4:A:764:HOH:O	1.93	0.68
1:H:174:GLU:OE1	1:H:201:LYS:HD3	1.94	0.67
3:A:502:DAO:H92	4:A:684:HOH:O	1.95	0.67
1:G:234:LEU:CD1	1:G:274:LEU:HB2	2.24	0.67
1:H:88:GLU:HG2	1:H:92:LYS:NZ	2.09	0.67
1:H:175:PRO:HG3	1:H:202:VAL:HG23	1.76	0.67
1:F:284:ILE:O	1:F:288:LEU:HD13	1.94	0.67
1:E:293:LEU:HD13	1:E:351:CYS:SG	2.35	0.66
1:G:234:LEU:HD11	1:G:274:LEU:HD22	1.75	0.66
1:F:417:ILE:O	1:F:421:LEU:HD23	1.94	0.66
1:G:318:LYS:HE2	4:G:715:HOH:O	1.95	0.66
1:H:76:HIS:O	1:H:80:GLU:HG3	1.95	0.66
1:G:99:LEU:O	1:G:110:ILE:HD13	1.96	0.66
1:A:138:SER:HA	1:A:142:MET:CE	2.25	0.65
1:A:172:MET:HG2	1:A:216:VAL:HG21	1.77	0.65
1:A:69:GLN:HB2	4:A:672:HOH:O	1.97	0.65
1:D:175:PRO:HG3	1:D:202:VAL:CG1	2.27	0.65
1:C:363:ALA:HB2	1:C:425:GLU:OE1	1.97	0.64
1:G:333:LYS:HE2	1:G:382:ASP:HB3	1.80	0.64
1:F:361:ASP:HB2	4:F:615:HOH:O	1.97	0.64
1:E:411:TYR:OH	3:E:502:DAO:H102	1.97	0.64
1:E:284:ILE:O	1:E:288:LEU:HD13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LYS:HD2	4:E:664:HOH:O	1.97	0.64
1:B:220:ASN:ND2	1:B:223:ALA:HB2	2.13	0.64
1:F:304:GLU:OE2	1:F:345:ARG:HD2	1.97	0.64
1:F:37:GLU:OE1	1:F:51:ARG:HG3	1.97	0.64
1:F:172:MET:HG2	1:F:216:VAL:HG21	1.80	0.64
1:A:284:ILE:O	1:A:288:LEU:HD13	1.97	0.63
1:A:292:ARG:HG3	1:A:292:ARG:NH1	2.11	0.63
1:B:104:ALA:HB3	1:B:107:LEU:HD12	1.80	0.63
1:B:358:LYS:HE3	4:B:789:HOH:O	1.97	0.63
1:D:293:LEU:HD21	1:D:352:LEU:HD23	1.79	0.63
1:B:288:LEU:O	1:B:292:ARG:HG3	1.99	0.63
1:D:60:PHE:O	1:D:64:VAL:HG23	1.98	0.63
1:C:69:GLN:HA	1:C:73:ILE:HD12	1.81	0.62
1:G:304:GLU:OE2	1:G:345:ARG:HD2	1.99	0.62
1:C:350:ASN:O	1:C:354:LEU:HD13	1.99	0.62
1:G:71:GLU:OE1	1:G:92:LYS:HE2	1.99	0.62
1:B:234:LEU:CD2	1:B:274:LEU:HB2	2.30	0.62
1:D:86:SER:O	1:D:89:VAL:HG12	1.99	0.62
1:E:329:THR:HG23	1:H:328:GLN:HG2	1.80	0.61
1:H:172:MET:HG2	1:H:216:VAL:HG21	1.81	0.61
1:H:104:ALA:HB3	1:H:107:LEU:HD12	1.81	0.61
1:A:64:VAL:HG23	1:A:123:GLU:HG3	1.82	0.61
1:D:175:PRO:HG3	1:D:202:VAL:HG11	1.83	0.61
1:A:174:GLU:HG2	1:A:201:LYS:HD3	1.82	0.61
1:B:428:PHE:O	1:B:429:ASP:HB3	2.01	0.61
1:H:99:LEU:O	1:H:110:ILE:HD13	2.00	0.61
1:E:208:SER:HB3	1:E:257:ASP:HB2	1.81	0.61
1:H:284:ILE:O	1:H:288:LEU:HG	2.00	0.60
1:C:171:ALA:HB1	1:C:201:LYS:HG3	1.82	0.60
1:H:289:PRO:HG2	4:H:631:HOH:O	2.01	0.60
1:D:102:ASN:HA	1:D:112:GLY:O	2.01	0.60
1:H:175:PRO:HG3	1:H:202:VAL:CG2	2.32	0.60
1:B:161:MET:CE	1:B:212:VAL:HG11	2.27	0.60
1:D:181:LEU:O	1:D:184:ILE:HG13	2.01	0.60
1:E:49:ILE:O	1:E:50:ARG:HB2	2.02	0.60
1:C:160:GLN:CG	1:C:166:CYS:HB2	2.32	0.60
1:C:424:ARG:HH11	1:C:424:ARG:HG2	1.64	0.59
1:G:289:PRO:HG2	4:G:654:HOH:O	2.02	0.59
3:D:502:DAO:H92	4:D:607:HOH:O	2.02	0.59
1:B:167:ILE:CD1	1:B:209:LEU:HD13	2.31	0.59
1:G:76:HIS:CD2	1:G:129:CYS:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HA	1:B:230:ILE:HD13	1.85	0.59
1:H:157:PHE:CE2	1:H:234:LEU:HD13	2.37	0.59
1:C:363:ALA:CB	1:C:425:GLU:OE1	2.50	0.59
1:G:110:ILE:CD1	1:G:162:THR:HG23	2.33	0.59
1:G:225:SER:HB3	1:G:228:HIS:ND1	2.18	0.59
1:A:104:ALA:HB3	1:A:107:LEU:HD12	1.84	0.58
1:A:286:LYS:NZ	4:A:601:HOH:O	2.35	0.58
1:F:171:ALA:HB1	1:F:201:LYS:HG3	1.86	0.58
1:A:304:GLU:OE2	1:A:345:ARG:HD2	2.03	0.58
1:B:304:GLU:OE2	1:B:345:ARG:HD2	2.02	0.58
1:F:181:LEU:HD12	1:F:184:ILE:HG21	1.84	0.58
1:G:157:PHE:CE2	1:G:234:LEU:HD23	2.39	0.58
1:H:151:GLU:O	1:H:155:LYS:HG3	2.04	0.58
1:G:49:ILE:O	1:G:50:ARG:HB2	2.03	0.58
1:C:181:LEU:O	1:C:181:LEU:HD23	2.03	0.58
1:E:56:GLU:HG3	4:E:842:HOH:O	2.02	0.58
1:C:312:ASN:HB3	4:C:603:HOH:O	2.04	0.58
1:H:304:GLU:OE2	1:H:345:ARG:HD2	2.03	0.58
1:B:188:ALA:HA	1:B:196:ILE:O	2.04	0.57
1:C:247:LYS:HZ2	1:C:247:LYS:CB	2.16	0.57
1:C:218:VAL:HA	1:C:230:ILE:HD13	1.85	0.57
1:D:49:ILE:O	1:D:50:ARG:HB2	2.05	0.57
1:H:220:ASN:HB3	1:H:229:GLY:HA2	1.86	0.57
1:A:411:TYR:OH	3:A:502:DAO:H102	2.05	0.56
1:E:406:ARG:NH1	1:E:409:PRO:HG2	2.21	0.56
1:G:95:LYS:O	1:G:95:LYS:HD3	2.04	0.56
1:F:411:TYR:OH	3:F:502:DAO:H102	2.06	0.56
1:D:277:GLU:HG2	1:D:278:ASN:ND2	2.20	0.56
1:H:110:ILE:CD1	1:H:162:THR:HG23	2.35	0.56
1:D:220:ASN:ND2	1:D:223:ALA:HB2	2.21	0.56
1:A:288:LEU:O	1:A:292:ARG:HG2	2.05	0.56
1:C:110:ILE:HD11	4:C:693:HOH:O	2.06	0.56
1:D:107:LEU:HD23	1:D:146:THR:HB	1.86	0.56
1:G:228:HIS:O	1:G:278:ASN:HB3	2.05	0.56
1:A:181:LEU:HD13	1:A:181:LEU:O	2.06	0.56
1:B:317:ARG:O	1:B:323:THR:HA	2.05	0.56
1:D:408:GLN:HB2	1:D:409:PRO:HD3	1.88	0.56
1:C:226:PRO:O	1:C:230:ILE:HG12	2.06	0.55
1:H:49:ILE:O	1:H:50:ARG:HB2	2.05	0.55
1:C:172:MET:HG2	1:C:216:VAL:HG21	1.88	0.55
1:H:150:SER:O	1:H:154:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:HA	1:B:155:LYS:HE3	1.88	0.55
1:A:181:LEU:HD22	1:A:184:ILE:HD11	1.87	0.55
1:B:49:ILE:O	1:B:50:ARG:HB2	2.07	0.55
1:D:243:ILE:HB	1:D:262:PHE:HB2	1.88	0.55
1:F:288:LEU:O	1:F:292:ARG:HG2	2.07	0.55
1:G:189:LYS:O	1:G:195:TRP:HA	2.07	0.55
1:H:34:GLU:HG3	1:H:35:ARG:HG3	1.88	0.55
1:A:181:LEU:HB2	4:A:811:HOH:O	2.05	0.55
1:G:95:LYS:HD3	1:G:95:LYS:C	2.27	0.55
1:F:49:ILE:O	1:F:50:ARG:HB2	2.07	0.55
1:H:42:LYS:HE2	4:H:789:HOH:O	2.05	0.55
1:H:42:LYS:HB3	1:H:46:ASP:OD2	2.06	0.55
1:A:50:ARG:HD2	1:A:349:ASP:OD2	2.06	0.54
1:B:100:GLY:O	1:B:103:ILE:HB	2.06	0.54
1:A:208:SER:HB3	1:A:257:ASP:HB2	1.89	0.54
1:C:225:SER:HB3	1:C:228:HIS:CE1	2.42	0.54
1:B:234:LEU:HD21	1:B:274:LEU:HB2	1.90	0.54
1:C:340:HIS:ND1	1:C:375:LEU:HD13	2.23	0.54
1:H:181:LEU:H	1:H:181:LEU:CD2	2.20	0.54
1:C:312:ASN:ND2	4:C:603:HOH:O	2.41	0.54
1:D:281:PHE:O	1:D:285:MET:HG2	2.08	0.54
3:F:502:DAO:H111	4:F:771:HOH:O	2.06	0.54
1:A:167:ILE:HD13	1:A:209:LEU:HD13	1.90	0.54
1:F:358:LYS:HE2	4:F:629:HOH:O	2.08	0.53
1:A:49:ILE:O	1:A:50:ARG:HB2	2.08	0.53
1:G:175:PRO:HG3	1:G:202:VAL:CG2	2.38	0.53
1:G:321:GLY:C	1:G:322:LYS:HG3	2.28	0.53
1:F:240:LYS:HE2	1:F:240:LYS:H	1.74	0.53
1:H:158:ILE:HB	1:H:159:PRO:HD3	1.91	0.53
1:G:175:PRO:HG3	1:G:202:VAL:HG21	1.90	0.53
1:G:234:LEU:HD13	1:G:274:LEU:HB2	1.88	0.53
1:E:190:LYS:HD2	1:E:192:GLY:O	2.09	0.53
2:B:501:FAD:H2A	4:B:648:HOH:O	2.10	0.52
1:G:110:ILE:HD11	1:G:162:THR:HG23	1.91	0.52
1:H:76:HIS:CD2	1:H:129:CYS:HB3	2.44	0.52
1:C:181:LEU:HD23	1:C:181:LEU:C	2.29	0.52
1:G:291:GLN:NE2	4:G:601:HOH:O	2.43	0.52
1:C:182:GLN:HB3	1:C:226:PRO:HG2	1.90	0.52
1:F:107:LEU:CD1	1:F:146:THR:HG23	2.40	0.52
1:G:202:VAL:HG12	1:G:203:PHE:N	2.25	0.52
1:B:240:LYS:HB2	1:B:240:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HB3	1:A:326:HIS:CD2	2.44	0.51
1:C:397:PRO:HB3	4:C:731:HOH:O	2.10	0.51
1:F:266:ILE:HG22	1:F:268:LEU:HD12	1.91	0.51
1:D:202:VAL:HG12	1:D:260:GLU:HG2	1.92	0.51
1:E:202:VAL:HG22	1:E:203:PHE:N	2.25	0.51
1:B:327:LEU:O	1:B:331:GLN:HG3	2.11	0.51
1:C:204:ILE:N	1:C:204:ILE:HD12	2.26	0.51
1:A:61:ARG:HA	1:A:64:VAL:HG22	1.93	0.51
1:C:411:TYR:OH	3:C:502:DAO:H102	2.11	0.51
1:G:86:SER:O	1:G:89:VAL:HG12	2.10	0.51
1:G:150:SER:OG	1:G:153:GLN:HG3	2.11	0.51
1:F:115:TYR:O	1:F:119:ILE:HG12	2.11	0.51
1:H:174:GLU:HG3	1:H:184:ILE:HA	1.92	0.51
1:H:281:PHE:O	1:H:285:MET:HG2	2.10	0.51
1:H:293:LEU:HD21	1:H:352:LEU:HD23	1.93	0.51
1:E:47:ILE:HG12	1:E:61:ARG:HG2	1.92	0.51
1:H:182:GLN:CG	1:H:226:PRO:HG3	2.37	0.51
1:C:76:HIS:CD2	1:C:129:CYS:HB3	2.46	0.50
1:E:65:ARG:O	1:E:69:GLN:HG3	2.10	0.50
1:H:202:VAL:HG12	1:H:203:PHE:N	2.25	0.50
1:A:291:GLN:OE1	3:A:502:DAO:H22	2.11	0.50
1:B:282:TYR:CZ	1:B:286:LYS:HD2	2.46	0.50
1:C:160:GLN:HG2	1:C:166:CYS:CB	2.41	0.50
1:C:190:LYS:HG3	1:C:194:ASP:O	2.12	0.50
1:D:58:ASP:O	1:D:61:ARG:HB3	2.11	0.50
1:F:240:LYS:HD3	1:F:240:LYS:N	2.26	0.50
1:H:47:ILE:HG12	1:H:61:ARG:HD2	1.92	0.50
1:A:97:GLY:HA2	4:A:682:HOH:O	2.11	0.50
1:B:99:LEU:O	1:B:110:ILE:HD13	2.10	0.50
1:B:226:PRO:O	1:B:230:ILE:HG12	2.12	0.50
1:H:95:LYS:HE2	4:H:776:HOH:O	2.11	0.50
1:D:181:LEU:O	1:D:181:LEU:HD23	2.12	0.50
1:E:136:ILE:HG13	4:E:681:HOH:O	2.12	0.50
1:A:181:LEU:HG	1:A:281:PHE:HE1	1.75	0.50
1:F:260:GLU:HG3	1:F:262:PHE:CE2	2.46	0.50
1:A:155:LYS:HD2	4:A:703:HOH:O	2.12	0.50
1:D:288:LEU:O	1:D:292:ARG:HG2	2.12	0.50
1:E:155:LYS:HD3	4:E:838:HOH:O	2.09	0.50
1:H:54:SER:HB2	1:H:55:PRO:HD2	1.94	0.50
1:D:168:GLY:HA2	1:D:212:VAL:O	2.12	0.50
1:B:76:HIS:CD2	1:B:129:CYS:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:LEU:O	1:G:114:LEU:HD22	2.11	0.49
1:H:140:ILE:HG21	1:H:170:ILE:HD13	1.93	0.49
1:B:219:THR:HG21	1:B:231:SER:HB2	1.94	0.49
1:G:73:ILE:N	1:G:74:PRO:HD2	2.27	0.49
1:H:267:ARG:NH1	1:H:267:ARG:HB2	2.27	0.49
1:C:160:GLN:CD	1:C:166:CYS:HB2	2.33	0.49
1:G:208:SER:HB3	1:G:257:ASP:HB2	1.94	0.49
1:H:88:GLU:HG2	1:H:92:LYS:HZ2	1.75	0.49
1:E:319:ALA:N	1:E:322:LYS:O	2.39	0.49
1:B:319:ALA:N	1:B:322:LYS:O	2.35	0.49
3:H:502:DAO:H111	4:H:634:HOH:O	2.13	0.49
1:C:49:ILE:O	1:C:50:ARG:HB2	2.12	0.49
1:D:87:ARG:HD2	4:D:618:HOH:O	2.12	0.49
1:A:64:VAL:CG2	1:A:123:GLU:HG3	2.42	0.49
1:A:202:VAL:HG22	1:A:203:PHE:N	2.27	0.49
1:D:34:GLU:OE1	1:D:34:GLU:HA	2.11	0.49
1:D:171:ALA:HA	1:D:204:ILE:HD12	1.93	0.49
1:F:54:SER:HB2	1:F:55:PRO:HD2	1.94	0.49
1:D:150:SER:O	1:D:154:ILE:HG13	2.12	0.49
1:G:158:ILE:HB	1:G:159:PRO:HD3	1.95	0.49
1:A:322:LYS:HB3	1:A:326:HIS:HD2	1.78	0.48
1:C:340:HIS:CE1	1:C:375:LEU:HD13	2.48	0.48
1:G:182:GLN:OE1	1:G:226:PRO:HG2	2.13	0.48
1:H:358:LYS:HD3	1:H:358:LYS:N	2.28	0.48
1:C:182:GLN:HB3	1:C:226:PRO:CG	2.44	0.48
1:A:156:HIS:CE1	1:G:224:PRO:HG3	2.49	0.48
1:H:136:ILE:HG23	1:H:170:ILE:HD12	1.95	0.48
1:D:411:TYR:OH	3:D:502:DAO:H102	2.13	0.48
1:E:101:VAL:HA	1:E:110:ILE:HG12	1.95	0.48
1:H:50:ARG:HD2	1:H:349:ASP:OD2	2.13	0.48
1:H:333:LYS:HB2	1:H:333:LYS:HE3	1.61	0.48
1:A:98:LEU:HD12	1:A:98:LEU:N	2.29	0.48
1:C:421:LEU:N	1:C:421:LEU:HD22	2.29	0.48
1:D:68:PHE:CD1	1:D:72:VAL:HG21	2.49	0.48
1:F:102:ASN:HA	1:F:112:GLY:O	2.13	0.48
1:C:218:VAL:HG22	1:C:230:ILE:HD11	1.95	0.48
1:H:136:ILE:HG23	1:H:170:ILE:CD1	2.44	0.48
1:E:226:PRO:O	1:E:230:ILE:HG12	2.14	0.48
1:H:65:ARG:O	1:H:69:GLN:HG3	2.14	0.48
1:F:421:LEU:HD12	4:F:779:HOH:O	2.13	0.48
1:A:122:GLU:HG2	1:A:301:SER:OG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:PRO:HG3	1:D:202:VAL:HG13	1.96	0.47
1:D:181:LEU:HD23	1:D:181:LEU:C	2.34	0.47
1:D:340:HIS:ND1	1:D:375:LEU:HD13	2.28	0.47
1:F:175:PRO:HG3	1:F:202:VAL:CG1	2.43	0.47
1:E:51:ARG:HD2	4:E:691:HOH:O	2.12	0.47
1:F:245:GLY:HA3	1:F:260:GLU:HG2	1.97	0.47
1:G:104:ALA:HB3	1:G:107:LEU:HD12	1.96	0.47
1:H:73:ILE:N	1:H:74:PRO:HD2	2.29	0.47
1:C:389:GLY:HA2	1:D:410:ILE:HG21	1.95	0.47
1:D:332:HIS:O	1:D:336:GLU:HG3	2.14	0.47
1:E:289:PRO:HG2	4:E:687:HOH:O	2.14	0.47
1:F:107:LEU:HD13	1:F:146:THR:HG23	1.96	0.47
1:A:148:HIS:HE1	1:A:286:LYS:HD3	1.79	0.47
1:F:174:GLU:HG2	1:F:201:LYS:HD3	1.97	0.47
1:F:340:HIS:ND1	1:F:375:LEU:HD13	2.29	0.47
1:G:69:GLN:HB3	4:G:821:HOH:O	2.13	0.47
1:B:428:PHE:O	1:B:429:ASP:CB	2.63	0.47
1:C:118:ALA:O	1:C:122:GLU:HG3	2.14	0.47
1:E:42:LYS:NZ	1:E:42:LYS:HB3	2.29	0.47
1:E:375:LEU:C	1:E:375:LEU:HD23	2.35	0.47
1:H:172:MET:HG2	1:H:216:VAL:CG2	2.45	0.47
1:A:340:HIS:ND1	1:A:375:LEU:HD13	2.29	0.47
1:B:202:VAL:HG22	1:B:203:PHE:N	2.30	0.47
1:C:319:ALA:O	1:C:322:LYS:O	2.32	0.47
1:D:34:GLU:HB3	1:D:35:ARG:H	1.57	0.47
1:F:205:SER:O	1:F:206:ASN:HB2	2.15	0.47
1:G:154:ILE:HG23	1:G:158:ILE:HG13	1.96	0.47
1:H:120:VAL:HG12	4:H:616:HOH:O	2.14	0.47
1:B:427:VAL:HG23	1:B:428:PHE:CD2	2.50	0.47
3:F:502:DAO:H92	4:F:794:HOH:O	2.14	0.47
1:G:171:ALA:HB1	1:G:201:LYS:HG3	1.97	0.47
1:B:158:ILE:HB	1:B:159:PRO:HD3	1.96	0.47
1:F:240:LYS:H	1:F:240:LYS:CE	2.28	0.47
1:A:172:MET:HG2	1:A:216:VAL:CG2	2.43	0.47
1:A:357:ALA:O	1:A:358:LYS:HB2	2.14	0.47
1:C:114:LEU:HD13	1:C:114:LEU:O	2.15	0.47
1:E:329:THR:CG2	1:H:328:GLN:HG2	2.43	0.46
1:F:286:LYS:HA	1:F:286:LYS:CE	2.43	0.46
1:A:154:ILE:HG23	1:A:158:ILE:HG13	1.96	0.46
1:B:135:SER:HB3	1:B:294:LEU:HD21	1.97	0.46
1:A:424:ARG:HD2	1:A:428:PHE:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ARG:O	1:D:69:GLN:HG3	2.14	0.46
1:D:292:ARG:HG3	1:D:292:ARG:NH1	2.19	0.46
1:A:414:THR:CG2	2:A:501:FAD:H5'2	2.46	0.46
1:F:397:PRO:HB3	4:F:705:HOH:O	2.16	0.46
1:F:172:MET:HG2	1:F:216:VAL:CG2	2.44	0.46
1:H:86:SER:O	1:H:89:VAL:HG12	2.15	0.46
1:E:181:LEU:HG	1:E:281:PHE:CE1	2.50	0.46
1:G:189:LYS:HB3	1:G:196:ILE:HB	1.98	0.46
1:B:284:ILE:O	1:B:288:LEU:HG	2.15	0.46
1:C:286:LYS:HE2	1:C:286:LYS:HA	1.98	0.46
1:D:136:ILE:HG13	4:D:686:HOH:O	2.15	0.46
1:H:39:PRO:HG3	1:H:342:CYS:HB3	1.98	0.46
1:B:225:SER:HB3	1:B:228:HIS:CE1	2.51	0.46
1:H:167:ILE:HG21	1:H:209:LEU:HD13	1.97	0.46
1:A:236:GLU:O	1:A:239:MET:HG3	2.15	0.46
1:D:69:GLN:O	1:D:74:PRO:HD3	2.16	0.46
1:C:225:SER:HB3	1:C:228:HIS:ND1	2.31	0.45
1:E:181:LEU:HG	1:E:281:PHE:HE1	1.80	0.45
1:F:104:ALA:HB3	1:F:107:LEU:HD12	1.98	0.45
1:E:142:MET:O	1:E:146:THR:HG23	2.16	0.45
1:H:88:GLU:HB2	4:H:723:HOH:O	2.16	0.45
1:B:425:GLU:OE1	1:B:425:GLU:HA	2.17	0.45
1:C:424:ARG:HH11	1:C:424:ARG:CG	2.27	0.45
1:D:292:ARG:HH11	1:D:292:ARG:CG	2.20	0.45
1:E:39:PRO:HG3	1:E:342:CYS:HB3	1.99	0.45
1:E:351:CYS:SG	1:E:360:LEU:CD1	3.05	0.45
1:G:103:ILE:HG23	1:G:146:THR:HG21	1.98	0.45
1:G:293:LEU:HD21	1:G:352:LEU:HD23	1.97	0.45
1:C:86:SER:O	1:C:89:VAL:HG12	2.16	0.45
1:F:96:GLN:HB3	1:F:98:LEU:CD1	2.44	0.45
1:F:425:GLU:HB2	4:F:687:HOH:O	2.17	0.45
1:G:67:PHE:HD1	1:G:96:GLN:OE1	2.00	0.45
1:A:96:GLN:HB3	1:A:98:LEU:CD1	2.46	0.45
1:C:284:ILE:O	1:C:288:LEU:HG	2.16	0.45
1:D:201:LYS:HB3	1:D:204:ILE:HD11	1.99	0.45
1:E:281:PHE:O	1:E:285:MET:HG2	2.17	0.45
1:F:319:ALA:O	1:F:322:LYS:O	2.34	0.45
1:H:344:THR:O	1:H:348:VAL:HG23	2.16	0.45
1:C:397:PRO:HG2	4:C:644:HOH:O	2.16	0.45
1:F:228:HIS:HA	4:F:793:HOH:O	2.17	0.45
1:F:370:TYR:OH	1:H:336:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:ALA:HB1	1:H:106:HIS:CE1	2.51	0.45
3:D:502:DAO:H111	4:D:718:HOH:O	2.16	0.45
1:E:152:GLU:HB2	4:E:778:HOH:O	2.17	0.45
1:F:62:LYS:HE2	4:F:831:HOH:O	2.17	0.45
1:G:323:THR:OG1	1:G:326:HIS:ND1	2.40	0.45
1:H:174:GLU:OE1	1:H:174:GLU:HA	2.16	0.45
1:A:96:GLN:HB3	1:A:98:LEU:HD13	1.98	0.45
1:A:226:PRO:HA	4:A:754:HOH:O	2.17	0.45
1:B:288:LEU:HD13	1:B:292:ARG:NH2	2.32	0.45
1:A:267:ARG:HG2	4:A:673:HOH:O	2.16	0.45
1:B:86:SER:O	1:B:89:VAL:HG12	2.17	0.45
1:B:171:ALA:HB1	1:B:201:LYS:HG3	1.99	0.45
1:D:104:ALA:HB3	1:D:107:LEU:HD22	1.98	0.45
1:F:118:ALA:O	1:F:122:GLU:HG3	2.17	0.45
1:H:103:ILE:CG2	1:H:146:THR:HG21	2.47	0.45
1:A:158:ILE:HB	1:A:159:PRO:HD3	1.99	0.44
1:B:122:GLU:HG2	1:B:301:SER:OG	2.16	0.44
1:B:167:ILE:HG21	1:B:209:LEU:CD1	2.47	0.44
1:D:147:ASN:HB3	1:D:148:HIS:CE1	2.52	0.44
1:D:170:ILE:HG23	1:D:170:ILE:O	2.17	0.44
1:F:55:PRO:HG2	1:F:56:GLU:OE1	2.17	0.44
1:G:288:LEU:N	1:G:289:PRO:HD2	2.32	0.44
1:A:173:THR:OG1	2:A:501:FAD:H1'1	2.17	0.44
1:B:182:GLN:HG3	1:B:226:PRO:CD	2.47	0.44
1:E:42:LYS:HB3	1:E:42:LYS:HZ2	1.81	0.44
1:H:171:ALA:HA	1:H:204:ILE:HD12	1.99	0.44
1:H:333:LYS:HD3	4:H:764:HOH:O	2.17	0.44
1:B:411:TYR:OH	3:B:502:DAO:H102	2.18	0.44
1:D:73:ILE:N	1:D:74:PRO:HD2	2.31	0.44
1:D:146:THR:HG23	1:D:158:ILE:HD11	2.00	0.44
1:D:297:ASP:HA	1:D:300:ILE:HG22	1.99	0.44
1:G:411:TYR:OH	3:G:502:DAO:H102	2.16	0.44
1:B:54:SER:HB2	1:B:55:PRO:HD2	1.99	0.44
1:D:376:GLN:OE1	1:D:408:GLN:HG3	2.18	0.44
1:E:188:ALA:HA	1:E:196:ILE:O	2.17	0.44
1:F:196:ILE:HD12	1:F:267:ARG:HG2	1.98	0.44
1:F:281:PHE:O	1:F:285:MET:HG2	2.17	0.44
1:A:51:ARG:NH2	1:C:354:LEU:CD1	2.80	0.44
1:D:173:THR:HG23	1:D:178:GLY:HA2	1.99	0.44
1:D:279:LYS:HB3	1:D:283:TYR:CE2	2.52	0.44
1:D:425:GLU:H	1:D:425:GLU:CD	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LYS:HD3	1:E:194:ASP:O	2.17	0.44
1:E:254:LYS:HE3	4:F:703:HOH:O	2.16	0.44
1:F:240:LYS:N	1:F:240:LYS:CD	2.81	0.44
1:G:157:PHE:O	1:G:161:MET:HG3	2.18	0.44
1:H:297:ASP:OD1	1:H:345:ARG:NH2	2.37	0.44
1:C:333:LYS:HE2	1:C:333:LYS:HA	1.98	0.44
1:E:181:LEU:O	1:E:184:ILE:HG12	2.17	0.44
1:G:159:PRO:HB2	4:G:765:HOH:O	2.18	0.44
1:A:181:LEU:O	1:A:184:ILE:HG13	2.18	0.44
1:B:277:GLU:O	1:B:278:ASN:HB2	2.18	0.44
1:C:83:GLY:HA3	1:C:247:LYS:HZ1	1.82	0.44
1:G:103:ILE:CG2	1:G:146:THR:HG21	2.48	0.44
1:G:201:LYS:O	1:G:260:GLU:HG3	2.18	0.44
1:H:87:ARG:HD3	4:H:656:HOH:O	2.17	0.44
1:B:182:GLN:HA	1:B:226:PRO:HG3	2.00	0.44
1:H:157:PHE:HE2	1:H:234:LEU:HD13	1.82	0.44
1:A:51:ARG:NH2	1:C:354:LEU:HD11	2.32	0.43
1:B:110:ILE:CD1	1:B:162:THR:HG23	2.48	0.43
1:D:47:ILE:HG23	1:D:61:ARG:HG2	2.00	0.43
1:A:167:ILE:CD1	1:A:209:LEU:HD13	2.47	0.43
1:A:181:LEU:HD13	1:A:181:LEU:C	2.39	0.43
1:C:62:LYS:NZ	4:C:606:HOH:O	2.51	0.43
1:D:102:ASN:HB2	1:D:117:ALA:HB2	2.00	0.43
1:F:292:ARG:HG3	1:F:292:ARG:NH1	2.30	0.43
1:H:414:THR:CG2	2:H:501:FAD:H5'2	2.48	0.43
1:B:323:THR:OG1	1:B:326:HIS:ND1	2.44	0.43
1:E:181:LEU:HD13	1:E:181:LEU:C	2.39	0.43
1:F:185:LYS:O	1:F:186:THR:C	2.56	0.43
1:G:359:ARG:HD3	4:G:732:HOH:O	2.19	0.43
1:B:282:TYR:O	1:B:286:LYS:HG3	2.18	0.43
1:C:114:LEU:HD13	1:C:114:LEU:C	2.38	0.43
1:C:202:VAL:O	1:C:204:ILE:HD12	2.18	0.43
1:D:169:ALA:HB3	1:D:213:VAL:HG22	2.00	0.43
1:G:110:ILE:HD11	4:G:603:HOH:O	2.17	0.43
1:G:414:THR:OG1	1:G:417:ILE:HG12	2.19	0.43
1:A:182:GLN:O	1:A:182:GLN:HG2	2.19	0.43
1:D:158:ILE:N	1:D:159:PRO:HD2	2.34	0.43
1:E:103:ILE:HB	1:E:109:GLY:HA3	2.00	0.43
1:E:155:LYS:HB3	4:E:828:HOH:O	2.18	0.43
1:E:288:LEU:N	1:E:289:PRO:HD2	2.33	0.43
1:E:370:TYR:OH	1:G:336:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HG12	1:C:330:VAL:HG21	2.00	0.43
1:D:414:THR:HG23	2:D:501:FAD:H5'2	2.01	0.43
1:H:118:ALA:O	1:H:122:GLU:HG3	2.19	0.43
1:H:294:LEU:HD22	3:H:502:DAO:H82	2.00	0.43
1:H:322:LYS:HD3	1:H:326:HIS:ND1	2.33	0.43
1:H:414:THR:HG23	4:H:626:HOH:O	2.18	0.43
1:A:277:GLU:O	1:A:278:ASN:HB2	2.19	0.43
1:A:322:LYS:HD3	1:A:326:HIS:CD2	2.54	0.43
1:B:225:SER:OG	1:B:226:PRO:HD2	2.19	0.43
1:C:118:ALA:HA	1:C:121:TRP:CE3	2.54	0.43
1:H:340:HIS:ND1	1:H:375:LEU:HD13	2.33	0.43
1:B:152:GLU:HA	1:B:155:LYS:CE	2.49	0.43
1:D:425:GLU:CD	1:D:425:GLU:N	2.72	0.43
1:F:121:TRP:CD2	1:F:294:LEU:HD13	2.54	0.43
1:G:88:GLU:OE2	1:G:92:LYS:HD2	2.19	0.43
1:H:103:ILE:HG23	1:H:146:THR:HG21	2.00	0.43
1:B:160:GLN:HG3	1:B:166:CYS:CB	2.49	0.43
1:B:288:LEU:HB3	1:B:292:ARG:NH1	2.34	0.43
1:D:118:ALA:HA	1:D:121:TRP:CE3	2.54	0.43
1:H:369:LYS:HD3	1:H:369:LYS:C	2.39	0.43
1:C:218:VAL:HG22	1:C:230:ILE:CD1	2.49	0.42
1:B:297:ASP:OD1	1:B:345:ARG:NH2	2.41	0.42
1:E:174:GLU:HG2	1:E:200:SER:O	2.18	0.42
1:F:260:GLU:HG2	4:F:602:HOH:O	2.19	0.42
1:G:236:GLU:O	1:G:239:MET:HG3	2.19	0.42
1:H:313:TYR:HA	1:H:316:GLN:OE1	2.18	0.42
1:C:196:ILE:CD1	1:C:267:ARG:HG2	2.48	0.42
1:D:186:THR:HG22	1:D:217:ALA:HB2	2.01	0.42
1:E:158:ILE:N	1:E:159:PRO:HD2	2.34	0.42
1:E:420:GLU:HG2	1:G:332:HIS:HE2	1.84	0.42
1:B:73:ILE:N	1:B:74:PRO:HD2	2.34	0.42
1:G:178:GLY:HA3	2:G:501:FAD:O2P	2.19	0.42
1:A:177:ALA:HB1	1:A:180:ASP:HB3	2.01	0.42
1:B:190:LYS:HE2	1:B:193:SER:HA	2.01	0.42
1:B:337:LEU:O	1:B:341:ILE:HG13	2.20	0.42
1:D:137:HIS:HE1	1:D:166:CYS:O	2.01	0.42
1:G:121:TRP:CE2	1:G:294:LEU:HD13	2.54	0.42
1:H:173:THR:OG1	2:H:501:FAD:H1'1	2.19	0.42
1:B:136:ILE:HD11	3:B:502:DAO:H41	2.02	0.42
1:F:69:GLN:HA	1:F:73:ILE:HD12	2.01	0.42
1:E:191:ASP:OD2	1:E:267:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:HA	1:A:204:ILE:HD12	2.01	0.42
1:B:137:HIS:HE1	1:B:166:CYS:O	2.03	0.42
1:C:281:PHE:O	1:C:285:MET:HG2	2.19	0.42
1:G:288:LEU:HD23	1:G:288:LEU:HA	1.86	0.42
1:H:395:GLU:HB2	4:H:627:HOH:O	2.20	0.42
1:C:101:VAL:HA	1:C:110:ILE:HB	2.01	0.42
1:C:136:ILE:HG12	3:C:502:DAO:H42	2.02	0.42
1:D:205:SER:O	1:D:206:ASN:HB2	2.19	0.42
1:E:61:ARG:HD3	1:E:123:GLU:OE2	2.19	0.42
1:E:100:GLY:HA3	1:E:162:THR:HG23	2.02	0.42
1:H:163:ALA:CB	1:H:165:LYS:HD3	2.50	0.42
1:A:427:VAL:O	1:A:427:VAL:HG22	2.19	0.42
1:D:77:SER:O	1:D:81:LYS:HG3	2.20	0.42
1:D:98:LEU:N	1:D:98:LEU:HD22	2.35	0.42
1:D:337:LEU:O	1:D:341:ILE:HG13	2.20	0.42
1:H:292:ARG:NH1	4:H:603:HOH:O	2.50	0.42
1:B:174:GLU:HG2	1:B:201:LYS:HD3	2.02	0.41
2:B:501:FAD:C2A	4:B:648:HOH:O	2.66	0.41
1:C:202:VAL:HG22	1:C:203:PHE:N	2.35	0.41
1:E:202:VAL:HG23	1:E:260:GLU:HG2	2.01	0.41
1:F:76:HIS:CD2	1:F:129:CYS:HB3	2.54	0.41
1:G:279:LYS:HE3	1:G:279:LYS:HB3	1.92	0.41
1:G:316:GLN:O	1:G:316:GLN:HG2	2.20	0.41
1:A:138:SER:HA	1:A:142:MET:HE3	2.01	0.41
1:A:193:SER:O	1:A:270:ALA:HB2	2.20	0.41
1:B:161:MET:HG2	1:B:166:CYS:O	2.20	0.41
1:E:151:GLU:O	1:E:155:LYS:HG3	2.20	0.41
1:F:175:PRO:HG3	1:F:202:VAL:HG11	2.01	0.41
1:G:234:LEU:HD11	1:G:274:LEU:HB2	2.00	0.41
1:H:140:ILE:HB	1:H:170:ILE:HD11	2.02	0.41
1:H:141:VAL:HG22	1:H:170:ILE:HG13	2.02	0.41
1:A:332:HIS:NE2	1:C:420:GLU:HG2	2.34	0.41
1:B:223:ALA:HB1	1:B:224:PRO:HD2	2.00	0.41
1:C:106:HIS:CE1	1:C:107:LEU:HG	2.55	0.41
1:D:47:ILE:HG12	1:D:61:ARG:HG2	2.02	0.41
1:D:182:GLN:O	1:D:182:GLN:HG2	2.20	0.41
1:F:414:THR:HG23	4:F:666:HOH:O	2.19	0.41
1:C:224:PRO:HG2	1:C:225:SER:H	1.85	0.41
1:F:181:LEU:HD12	1:F:184:ILE:CG2	2.49	0.41
1:H:243:ILE:HB	1:H:262:PHE:HB2	2.01	0.41
1:D:106:HIS:CE1	1:D:107:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:GLU:O	1:E:278:ASN:HB2	2.21	0.41
1:F:118:ALA:HA	1:F:121:TRP:CE3	2.55	0.41
1:G:136:ILE:HG12	3:G:502:DAO:H42	2.01	0.41
1:A:76:HIS:CD2	1:A:129:CYS:HB3	2.55	0.41
1:B:293:LEU:HD21	1:B:352:LEU:HD23	2.02	0.41
1:C:61:ARG:HD2	1:C:123:GLU:OE2	2.21	0.41
1:C:85:VAL:HG22	4:C:619:HOH:O	2.20	0.41
1:D:39:PRO:HG3	1:D:342:CYS:HB3	2.03	0.41
1:H:65:ARG:HD3	1:H:123:GLU:OE1	2.21	0.41
1:H:76:HIS:HB3	4:H:765:HOH:O	2.21	0.41
1:H:357:ALA:HB1	4:H:703:HOH:O	2.20	0.41
1:A:205:SER:O	1:A:206:ASN:HB2	2.21	0.41
1:A:381:TYR:OH	1:B:374:GLU:OE2	2.32	0.41
1:B:79:TRP:CG	1:B:85:VAL:HA	2.56	0.41
1:B:340:HIS:CG	1:B:375:LEU:HD12	2.55	0.41
1:B:369:LYS:HD3	1:B:369:LYS:C	2.41	0.41
1:C:246:ARG:HB3	1:C:246:ARG:NH1	2.35	0.41
1:E:179:SER:HB3	1:E:417:ILE:HD11	2.01	0.41
1:E:414:THR:CG2	2:E:501:FAD:H5'2	2.50	0.41
1:B:155:LYS:HA	4:B:760:HOH:O	2.20	0.41
1:E:268:LEU:HA	1:E:269:PRO:HD3	1.92	0.41
1:G:322:LYS:HD2	4:G:818:HOH:O	2.19	0.41
1:A:152:GLU:HG3	1:G:228:HIS:HE2	1.86	0.41
1:B:182:GLN:N	1:B:182:GLN:OE1	2.53	0.41
1:B:222:GLU:HB3	4:B:704:HOH:O	2.20	0.41
1:B:375:LEU:C	1:B:375:LEU:HD23	2.42	0.41
1:C:210:SER:O	1:C:244:LYS:NZ	2.50	0.41
1:D:79:TRP:CG	1:D:85:VAL:HA	2.56	0.41
1:D:186:THR:HG22	1:D:217:ALA:CB	2.51	0.41
1:D:375:LEU:O	1:D:379:VAL:HG23	2.21	0.41
1:E:322:LYS:HE2	4:E:678:HOH:O	2.21	0.41
3:F:502:DAO:H111	4:F:841:HOH:O	2.20	0.41
1:H:110:ILE:N	1:H:110:ILE:HD12	2.36	0.41
1:H:119:ILE:O	1:H:123:GLU:HG2	2.21	0.41
1:H:206:ASN:O	1:H:210:SER:HB3	2.19	0.41
1:A:137:HIS:CD2	1:A:142:MET:HE2	2.56	0.41
1:E:102:ASN:HD22	1:E:102:ASN:HA	1.67	0.41
1:A:54:SER:HB2	1:A:55:PRO:HD2	2.02	0.40
1:A:369:LYS:HD3	1:A:369:LYS:C	2.41	0.40
1:B:104:ALA:HB1	1:B:106:HIS:CE1	2.56	0.40
1:D:424:ARG:HB3	1:D:425:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:LEU:HD12	1:F:268:LEU:N	2.36	0.40
1:F:333:LYS:HD3	4:F:673:HOH:O	2.21	0.40
1:A:61:ARG:O	1:A:64:VAL:HG22	2.22	0.40
1:A:414:THR:HG23	2:A:501:FAD:H5'2	2.04	0.40
1:D:292:ARG:NH1	1:D:292:ARG:CG	2.80	0.40
1:H:375:LEU:O	1:H:379:VAL:HG23	2.21	0.40
1:C:172:MET:HG2	1:C:216:VAL:CG2	2.51	0.40
1:D:92:LYS:O	1:D:96:GLN:HG3	2.22	0.40
1:D:167:ILE:O	1:D:210:SER:HA	2.22	0.40
1:D:369:LYS:HD3	1:D:369:LYS:C	2.42	0.40
1:G:69:GLN:HA	1:G:73:ILE:HD12	2.03	0.40
1:A:73:ILE:N	1:A:74:PRO:HD2	2.37	0.40
1:A:309:GLU:OE2	1:A:397:PRO:HG2	2.22	0.40
1:C:294:LEU:HD23	1:C:294:LEU:C	2.42	0.40
1:F:136:ILE:HD11	3:F:502:DAO:H41	2.04	0.40
1:B:118:ALA:HA	1:B:121:TRP:CE3	2.56	0.40
1:D:231:SER:HB2	1:D:233:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/400 (98%)	384 (98%)	9 (2%)	0	100	100
1	B	394/400 (98%)	385 (98%)	8 (2%)	1 (0%)	41	37
1	C	393/400 (98%)	386 (98%)	6 (2%)	1 (0%)	41	37
1	D	393/400 (98%)	380 (97%)	13 (3%)	0	100	100
1	E	393/400 (98%)	385 (98%)	7 (2%)	1 (0%)	41	37
1	F	394/400 (98%)	385 (98%)	8 (2%)	1 (0%)	41	37
1	G	394/400 (98%)	384 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	393/400 (98%)	385 (98%)	8 (2%)	0	100 100
All	All	3147/3200 (98%)	3074 (98%)	69 (2%)	4 (0%)	51 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	ARG
1	B	50	ARG
1	E	50	ARG
1	F	50	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	325/328 (99%)	319 (98%)	6 (2%)	59 63
1	B	326/328 (99%)	318 (98%)	8 (2%)	47 49
1	C	325/328 (99%)	318 (98%)	7 (2%)	52 55
1	D	325/328 (99%)	319 (98%)	6 (2%)	59 63
1	E	325/328 (99%)	318 (98%)	7 (2%)	52 55
1	F	326/328 (99%)	318 (98%)	8 (2%)	47 49
1	G	326/328 (99%)	319 (98%)	7 (2%)	53 57
1	H	325/328 (99%)	316 (97%)	9 (3%)	43 44
All	All	2603/2624 (99%)	2545 (98%)	58 (2%)	52 55

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	256	GLN
1	A	316	GLN
1	A	333	LYS

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Mol	Chain	Res	Type
1	A	350	ASN
1	A	411	TYR
1	B	182	GLN
1	B	228	HIS
1	B	256	GLN
1	B	312	ASN
1	B	350	ASN
1	B	370	TYR
1	B	411	TYR
1	B	420	GLU
1	C	69	GLN
1	C	256	GLN
1	C	312	ASN
1	C	333	LYS
1	C	350	ASN
1	C	370	TYR
1	C	411	TYR
1	D	34	GLU
1	D	256	GLN
1	D	323	THR
1	D	350	ASN
1	D	370	TYR
1	D	411	TYR
1	E	61	ARG
1	E	102	ASN
1	E	256	GLN
1	E	333	LYS
1	E	350	ASN
1	E	370	TYR
1	E	411	TYR
1	F	96	GLN
1	F	256	GLN
1	F	279	LYS
1	F	316	GLN
1	F	350	ASN
1	F	361	ASP
1	F	370	TYR
1	F	411	TYR
1	G	95	LYS
1	G	256	GLN
1	G	316	GLN
1	G	350	ASN

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Mol	Chain	Res	Type
1	G	370	TYR
1	G	411	TYR
1	G	420	GLU
1	H	65	ARG
1	H	114	LEU
1	H	198	ASN
1	H	209	LEU
1	H	256	GLN
1	H	316	GLN
1	H	350	ASN
1	H	370	TYR
1	H	411	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	HIS
1	E	102	ASN
1	F	316	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	F	501	-	53,58,58	1.94	10 (18%)	68,89,89	1.61	14 (20%)
2	FAD	A	501	-	53,58,58	1.94	10 (18%)	68,89,89	1.61	15 (22%)
3	DAO	G	502	-	13,13,13	0.68	0	13,13,13	1.07	0
3	DAO	H	502	-	13,13,13	0.69	0	13,13,13	1.09	0
3	DAO	C	502	-	13,13,13	0.69	0	13,13,13	1.12	1 (7%)
2	FAD	B	501	-	53,58,58	1.94	10 (18%)	68,89,89	1.59	15 (22%)
2	FAD	D	501	-	53,58,58	1.95	10 (18%)	68,89,89	1.63	15 (22%)
3	DAO	D	502	-	13,13,13	0.69	0	13,13,13	1.12	0
2	FAD	H	501	-	53,58,58	1.95	10 (18%)	68,89,89	1.63	15 (22%)
3	DAO	E	502	-	13,13,13	0.69	0	13,13,13	1.08	0
3	DAO	B	502	-	13,13,13	0.69	0	13,13,13	1.09	0
3	DAO	A	502	-	13,13,13	0.70	0	13,13,13	1.10	0
2	FAD	E	501	-	53,58,58	1.95	10 (18%)	68,89,89	1.59	14 (20%)
2	FAD	G	501	-	53,58,58	1.94	10 (18%)	68,89,89	1.60	15 (22%)
2	FAD	C	501	-	53,58,58	1.95	10 (18%)	68,89,89	1.61	15 (22%)
3	DAO	F	502	-	13,13,13	0.69	0	13,13,13	1.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	501	-	-	0/30/50/50	0/6/6/6
2	FAD	A	501	-	-	0/30/50/50	0/6/6/6
3	DAO	G	502	-	-	2/11/11/11	-
3	DAO	H	502	-	-	0/11/11/11	-
3	DAO	C	502	-	-	2/11/11/11	-
2	FAD	B	501	-	-	0/30/50/50	0/6/6/6
2	FAD	D	501	-	-	1/30/50/50	0/6/6/6
3	DAO	D	502	-	-	0/11/11/11	-
2	FAD	H	501	-	-	2/30/50/50	0/6/6/6
3	DAO	E	502	-	-	0/11/11/11	-
3	DAO	B	502	-	-	0/11/11/11	-
3	DAO	A	502	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	E	501	-	-	0/30/50/50	0/6/6/6
2	FAD	G	501	-	-	2/30/50/50	0/6/6/6
2	FAD	C	501	-	-	0/30/50/50	0/6/6/6
3	DAO	F	502	-	-	2/11/11/11	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FAD	C8M-C8	-5.79	1.39	1.51
2	A	501	FAD	C7M-C7	-5.77	1.39	1.51
2	H	501	FAD	C7M-C7	-5.77	1.39	1.51
2	G	501	FAD	C8M-C8	-5.76	1.39	1.51
2	H	501	FAD	C8M-C8	-5.76	1.39	1.51
2	C	501	FAD	C8M-C8	-5.75	1.39	1.51
2	D	501	FAD	C7M-C7	-5.75	1.39	1.51
2	A	501	FAD	C8M-C8	-5.75	1.39	1.51
2	D	501	FAD	C8M-C8	-5.75	1.39	1.51
2	F	501	FAD	C7M-C7	-5.74	1.39	1.51
2	G	501	FAD	C7M-C7	-5.74	1.39	1.51
2	C	501	FAD	C7M-C7	-5.74	1.39	1.51
2	B	501	FAD	C7M-C7	-5.73	1.39	1.51
2	F	501	FAD	C8M-C8	-5.73	1.39	1.51
2	E	501	FAD	C7M-C7	-5.72	1.39	1.51
2	B	501	FAD	C8M-C8	-5.71	1.39	1.51
2	B	501	FAD	C2A-N3A	5.17	1.40	1.32
2	E	501	FAD	C2A-N3A	5.16	1.40	1.32
2	D	501	FAD	C2A-N3A	5.15	1.40	1.32
2	H	501	FAD	C2A-N3A	5.15	1.40	1.32
2	F	501	FAD	C2A-N3A	5.14	1.40	1.32
2	A	501	FAD	C2A-N3A	5.12	1.40	1.32
2	G	501	FAD	C2A-N3A	5.12	1.40	1.32
2	C	501	FAD	C2A-N3A	5.11	1.40	1.32
2	C	501	FAD	C4X-N5	5.00	1.40	1.30
2	A	501	FAD	C4X-N5	4.98	1.40	1.30
2	B	501	FAD	C4X-N5	4.97	1.40	1.30
2	E	501	FAD	C4X-N5	4.97	1.40	1.30
2	H	501	FAD	C4X-N5	4.97	1.40	1.30
2	F	501	FAD	C4X-N5	4.97	1.40	1.30
2	D	501	FAD	C4X-N5	4.97	1.40	1.30
2	G	501	FAD	C4X-N5	4.97	1.40	1.30
2	B	501	FAD	C9A-N10	-3.69	1.34	1.41
2	C	501	FAD	C9A-N10	-3.67	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	FAD	C9A-N10	-3.67	1.34	1.41
2	D	501	FAD	C9A-N10	-3.66	1.34	1.41
2	H	501	FAD	C9A-N10	-3.65	1.34	1.41
2	F	501	FAD	C9A-N10	-3.64	1.34	1.41
2	E	501	FAD	C9A-N10	-3.61	1.34	1.41
2	B	501	FAD	C10-N1	3.61	1.40	1.33
2	E	501	FAD	C10-N1	3.60	1.40	1.33
2	A	501	FAD	C9A-N10	-3.59	1.34	1.41
2	G	501	FAD	C10-N1	3.59	1.40	1.33
2	A	501	FAD	C10-N1	3.58	1.40	1.33
2	H	501	FAD	C10-N1	3.56	1.40	1.33
2	C	501	FAD	C10-N1	3.55	1.40	1.33
2	F	501	FAD	C10-N1	3.55	1.40	1.33
2	D	501	FAD	C10-N1	3.54	1.40	1.33
2	G	501	FAD	C2A-N1A	3.51	1.40	1.33
2	D	501	FAD	C2A-N1A	3.50	1.40	1.33
2	H	501	FAD	C2A-N1A	3.48	1.40	1.33
2	B	501	FAD	C2A-N1A	3.47	1.40	1.33
2	C	501	FAD	C2A-N1A	3.45	1.40	1.33
2	E	501	FAD	C2A-N1A	3.45	1.40	1.33
2	A	501	FAD	C2A-N1A	3.45	1.40	1.33
2	F	501	FAD	C2A-N1A	3.43	1.40	1.33
2	E	501	FAD	C5A-C4A	-2.78	1.33	1.40
2	C	501	FAD	C5A-C4A	-2.78	1.33	1.40
2	F	501	FAD	C5A-C4A	-2.77	1.33	1.40
2	H	501	FAD	C5A-C4A	-2.77	1.33	1.40
2	D	501	FAD	C5A-C4A	-2.76	1.33	1.40
2	G	501	FAD	C5A-C4A	-2.75	1.33	1.40
2	A	501	FAD	C5A-C4A	-2.75	1.33	1.40
2	B	501	FAD	C5A-C4A	-2.74	1.33	1.40
2	C	501	FAD	C6A-C5A	-2.63	1.33	1.43
2	B	501	FAD	C6A-C5A	-2.63	1.33	1.43
2	E	501	FAD	C6A-C5A	-2.63	1.33	1.43
2	D	501	FAD	C6A-C5A	-2.62	1.33	1.43
2	H	501	FAD	C6A-C5A	-2.62	1.33	1.43
2	F	501	FAD	C6A-C5A	-2.61	1.33	1.43
2	A	501	FAD	C6A-C5A	-2.60	1.33	1.43
2	G	501	FAD	C6A-C5A	-2.59	1.33	1.43
2	F	501	FAD	O4B-C1B	2.29	1.44	1.41
2	H	501	FAD	O4B-C1B	2.26	1.44	1.41
2	G	501	FAD	O4B-C1B	2.25	1.44	1.41
2	E	501	FAD	O4B-C1B	2.22	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	O4B-C1B	2.21	1.44	1.41
2	A	501	FAD	O4B-C1B	2.21	1.44	1.41
2	B	501	FAD	O4B-C1B	2.20	1.44	1.41
2	C	501	FAD	O4B-C1B	2.18	1.44	1.41

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	N3A-C2A-N1A	-6.94	117.83	128.68
2	F	501	FAD	N3A-C2A-N1A	-6.93	117.84	128.68
2	H	501	FAD	N3A-C2A-N1A	-6.93	117.85	128.68
2	D	501	FAD	N3A-C2A-N1A	-6.93	117.85	128.68
2	G	501	FAD	N3A-C2A-N1A	-6.91	117.87	128.68
2	E	501	FAD	N3A-C2A-N1A	-6.90	117.89	128.68
2	C	501	FAD	N3A-C2A-N1A	-6.88	117.93	128.68
2	B	501	FAD	N3A-C2A-N1A	-6.84	117.98	128.68
2	E	501	FAD	P-O3P-PA	-3.54	120.67	132.83
2	H	501	FAD	P-O3P-PA	-3.47	120.93	132.83
2	G	501	FAD	P-O3P-PA	-3.45	121.00	132.83
2	A	501	FAD	P-O3P-PA	-3.39	121.19	132.83
2	F	501	FAD	P-O3P-PA	-3.36	121.30	132.83
2	D	501	FAD	P-O3P-PA	-3.32	121.45	132.83
2	B	501	FAD	P-O3P-PA	-3.26	121.63	132.83
2	C	501	FAD	P-O3P-PA	-3.21	121.81	132.83
2	H	501	FAD	C4-N3-C2	-3.16	119.80	125.64
2	A	501	FAD	C4-N3-C2	-3.14	119.85	125.64
2	F	501	FAD	C4-N3-C2	-3.12	119.88	125.64
2	D	501	FAD	C4-N3-C2	-3.11	119.89	125.64
2	B	501	FAD	C4-N3-C2	-3.10	119.91	125.64
2	D	501	FAD	O4B-C1B-C2B	-3.10	102.39	106.93
2	E	501	FAD	C4-N3-C2	-3.10	119.92	125.64
2	G	501	FAD	C4-N3-C2	-3.10	119.92	125.64
2	C	501	FAD	C4-N3-C2	-3.05	120.01	125.64
2	F	501	FAD	C9A-C5X-N5	-3.01	119.16	122.43
2	C	501	FAD	C4X-C10-N10	2.99	120.85	116.48
2	C	501	FAD	C9A-C5X-N5	-2.98	119.19	122.43
2	G	501	FAD	C9A-C5X-N5	-2.94	119.24	122.43
2	E	501	FAD	C4X-C10-N10	2.92	120.75	116.48
2	H	501	FAD	C9A-C5X-N5	-2.91	119.27	122.43
2	B	501	FAD	C9A-C5X-N5	-2.90	119.28	122.43
2	A	501	FAD	C9A-C5X-N5	-2.90	119.28	122.43
2	H	501	FAD	C4X-C10-N10	2.90	120.72	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	FAD	C4X-C10-N10	2.89	120.70	116.48
2	B	501	FAD	C4X-C10-N10	2.86	120.66	116.48
2	D	501	FAD	C3B-C2B-C1B	-2.85	96.68	100.98
2	D	501	FAD	C9A-C5X-N5	-2.85	119.34	122.43
2	D	501	FAD	C4X-C10-N10	2.84	120.64	116.48
2	G	501	FAD	C4X-C10-N10	2.84	120.63	116.48
2	H	501	FAD	O4B-C1B-C2B	-2.83	102.78	106.93
2	E	501	FAD	C9A-C5X-N5	-2.82	119.37	122.43
2	C	501	FAD	C10-C4X-N5	-2.81	118.90	124.86
2	A	501	FAD	C4X-C10-N10	2.80	120.58	116.48
2	C	501	FAD	O4B-C1B-C2B	-2.77	102.87	106.93
2	B	501	FAD	O4B-C1B-C2B	-2.74	102.92	106.93
2	H	501	FAD	C4X-C4-N3	2.74	120.14	113.19
2	F	501	FAD	C10-C4X-N5	-2.73	119.07	124.86
2	F	501	FAD	C5A-C6A-N6A	-2.72	116.22	120.35
2	A	501	FAD	C5A-C6A-N6A	-2.72	116.22	120.35
2	F	501	FAD	C4X-C4-N3	2.71	120.08	113.19
2	H	501	FAD	C5A-C6A-N6A	-2.71	116.24	120.35
2	H	501	FAD	C10-C4X-N5	-2.70	119.13	124.86
2	D	501	FAD	C5A-C6A-N6A	-2.69	116.27	120.35
2	E	501	FAD	C5A-C6A-N6A	-2.69	116.27	120.35
2	D	501	FAD	C4X-C4-N3	2.68	120.00	113.19
2	A	501	FAD	C4X-C4-N3	2.68	119.98	113.19
2	C	501	FAD	C4X-C4-N3	2.67	119.98	113.19
2	A	501	FAD	C10-C4X-N5	-2.67	119.19	124.86
2	E	501	FAD	C10-C4X-N5	-2.67	119.19	124.86
2	G	501	FAD	C10-C4X-N5	-2.67	119.20	124.86
2	A	501	FAD	O4B-C1B-C2B	-2.66	103.04	106.93
2	B	501	FAD	C10-C4X-N5	-2.66	119.22	124.86
2	D	501	FAD	C10-C4X-N5	-2.65	119.23	124.86
2	B	501	FAD	C4X-C4-N3	2.64	119.89	113.19
2	G	501	FAD	C4X-C4-N3	2.64	119.89	113.19
2	F	501	FAD	O4B-C1B-C2B	-2.64	103.07	106.93
2	E	501	FAD	C4X-C4-N3	2.61	119.83	113.19
2	B	501	FAD	C5X-C9A-N10	2.59	120.63	117.95
2	F	501	FAD	C5X-C9A-N10	2.58	120.61	117.95
2	E	501	FAD	C5X-C9A-N10	2.55	120.59	117.95
2	G	501	FAD	C5A-C6A-N6A	-2.55	116.48	120.35
2	C	501	FAD	C5A-C6A-N6A	-2.54	116.49	120.35
2	G	501	FAD	C5X-C9A-N10	2.54	120.58	117.95
2	B	501	FAD	C5A-C6A-N6A	-2.54	116.50	120.35
2	C	501	FAD	C5X-C9A-N10	2.53	120.57	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	C5X-C9A-N10	2.51	120.55	117.95
2	D	501	FAD	C5X-C9A-N10	2.51	120.55	117.95
2	G	501	FAD	C3B-C2B-C1B	-2.51	97.20	100.98
2	H	501	FAD	C5X-C9A-N10	2.51	120.54	117.95
2	C	501	FAD	C3B-C2B-C1B	-2.51	97.21	100.98
2	G	501	FAD	O4B-C1B-C2B	-2.47	103.31	106.93
2	H	501	FAD	C3B-C2B-C1B	-2.46	97.27	100.98
2	E	501	FAD	C4-C4X-C10	2.45	120.90	116.79
2	B	501	FAD	C4-C4X-C10	2.41	120.84	116.79
2	A	501	FAD	C3B-C2B-C1B	-2.39	97.38	100.98
2	A	501	FAD	C4-C4X-C10	2.36	120.76	116.79
2	E	501	FAD	C4X-C10-N1	-2.35	119.28	124.73
2	E	501	FAD	O4B-C1B-C2B	-2.35	103.50	106.93
2	A	501	FAD	C4X-C10-N1	-2.34	119.30	124.73
2	G	501	FAD	C4-C4X-C10	2.34	120.72	116.79
2	B	501	FAD	C3B-C2B-C1B	-2.32	97.49	100.98
2	F	501	FAD	C3B-C2B-C1B	-2.31	97.50	100.98
2	B	501	FAD	C4X-C10-N1	-2.31	119.38	124.73
2	F	501	FAD	C4X-C10-N1	-2.31	119.38	124.73
2	H	501	FAD	C4X-C10-N1	-2.29	119.41	124.73
2	D	501	FAD	O4-C4-C4X	-2.29	120.51	126.60
2	D	501	FAD	C4-C4X-C10	2.29	120.64	116.79
2	B	501	FAD	O4-C4-C4X	-2.29	120.53	126.60
2	F	501	FAD	C4-C4X-C10	2.29	120.63	116.79
2	G	501	FAD	O4-C4-C4X	-2.26	120.60	126.60
2	C	501	FAD	C4-C4X-C10	2.24	120.56	116.79
2	H	501	FAD	C4-C4X-C10	2.24	120.56	116.79
2	C	501	FAD	C4X-C10-N1	-2.24	119.53	124.73
2	G	501	FAD	C4X-C10-N1	-2.24	119.54	124.73
2	C	501	FAD	O4-C4-C4X	-2.23	120.70	126.60
2	D	501	FAD	C4X-C10-N1	-2.22	119.58	124.73
2	E	501	FAD	O4-C4-C4X	-2.22	120.71	126.60
2	H	501	FAD	O4-C4-C4X	-2.22	120.71	126.60
2	A	501	FAD	O4-C4-C4X	-2.21	120.73	126.60
2	F	501	FAD	O4-C4-C4X	-2.13	120.96	126.60
2	C	501	FAD	O2A-PA-O1A	2.08	122.53	112.24
3	C	502	DAO	C3-C2-C1	-2.06	109.29	114.47
2	A	501	FAD	O2A-PA-O1A	2.05	122.37	112.24
2	E	501	FAD	O2A-PA-O1A	2.05	122.36	112.24
2	H	501	FAD	O2A-PA-O1A	2.05	122.36	112.24
2	B	501	FAD	O2A-PA-O1A	2.05	122.35	112.24
2	G	501	FAD	O2A-PA-O1A	2.04	122.35	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FAD	O2A-PA-O1A	2.04	122.30	112.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	501	FAD	PA-O3P-P-O1P
2	H	501	FAD	PA-O3P-P-O1P
3	F	502	DAO	O1-C1-C2-C3
3	A	502	DAO	O1-C1-C2-C3
3	C	502	DAO	O1-C1-C2-C3
3	F	502	DAO	O2-C1-C2-C3
3	G	502	DAO	O2-C1-C2-C3
3	G	502	DAO	O1-C1-C2-C3
2	D	501	FAD	PA-O3P-P-O2P
2	G	501	FAD	PA-O3P-P-O2P
2	H	501	FAD	PA-O3P-P-O2P
3	A	502	DAO	O2-C1-C2-C3
3	C	502	DAO	O2-C1-C2-C3

There are no ring outliers.

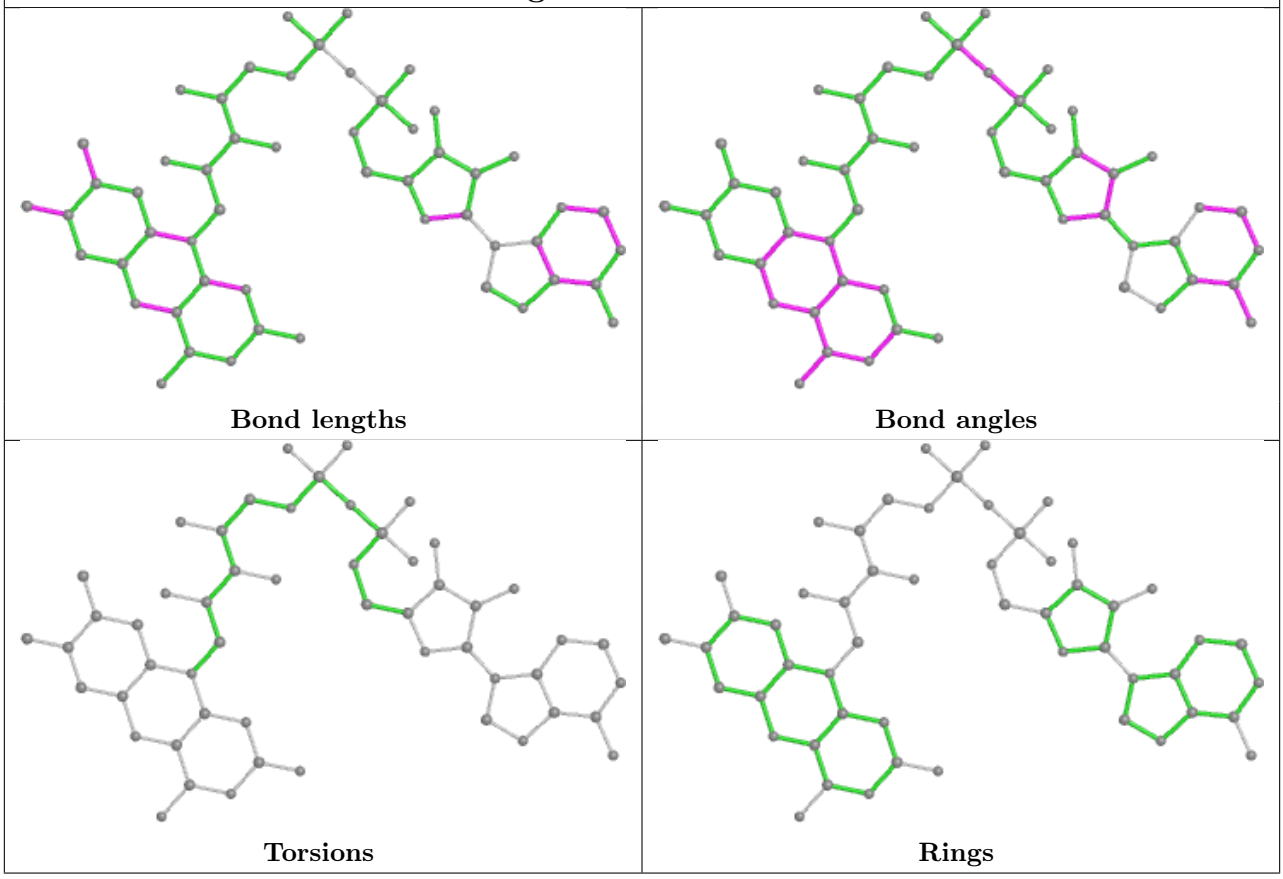
14 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	3	0
3	G	502	DAO	2	0
3	H	502	DAO	2	0
3	C	502	DAO	2	0
2	B	501	FAD	2	0
2	D	501	FAD	1	0
3	D	502	DAO	3	0
2	H	501	FAD	2	0
3	E	502	DAO	2	0
3	B	502	DAO	2	0
3	A	502	DAO	3	0
2	E	501	FAD	1	0
2	G	501	FAD	1	0
3	F	502	DAO	5	0

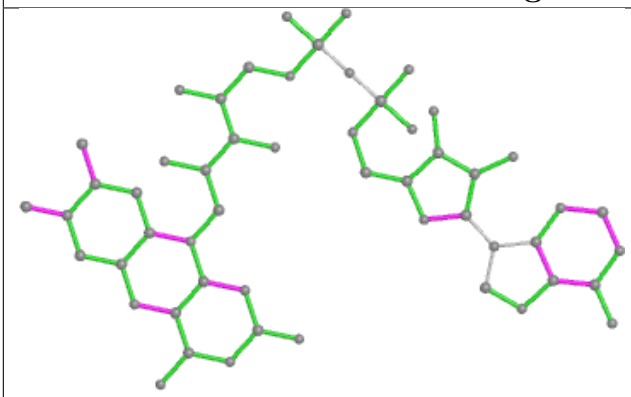
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

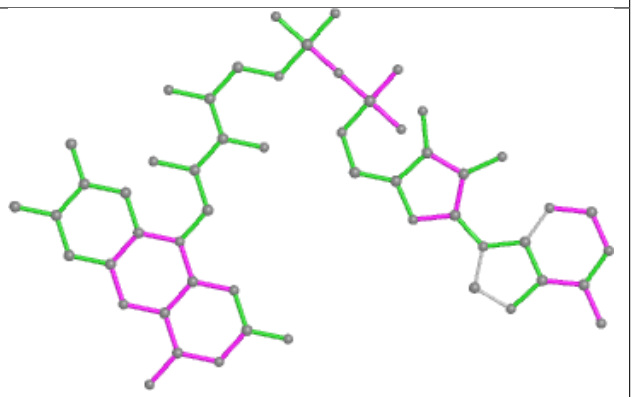
Ligand FAD F 501



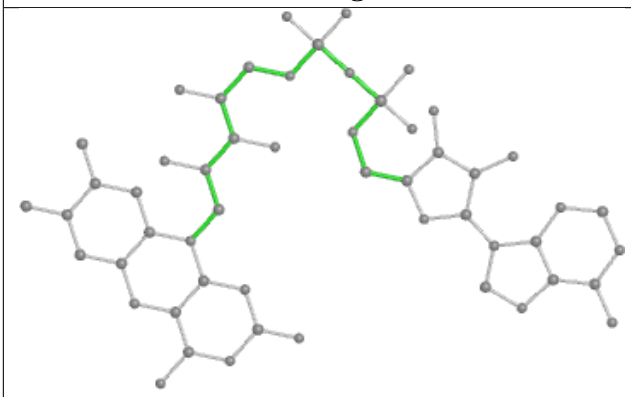
Ligand FAD A 501



Bond lengths



Bond angles



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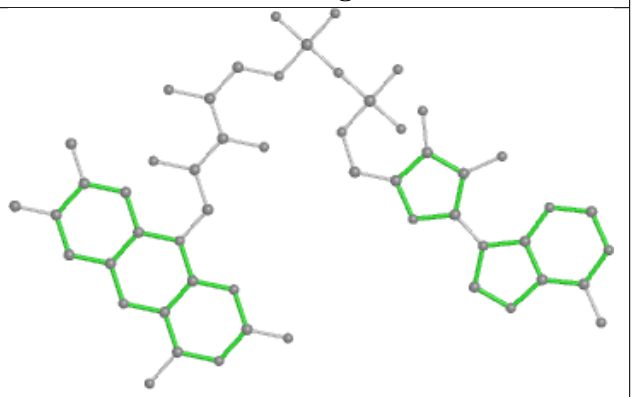
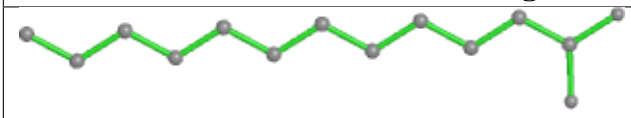


Rings

Ligand DAO G 502



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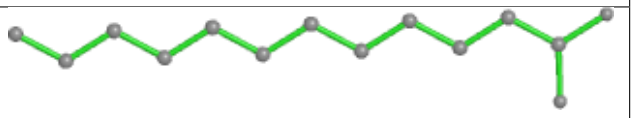

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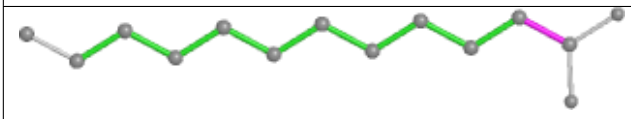

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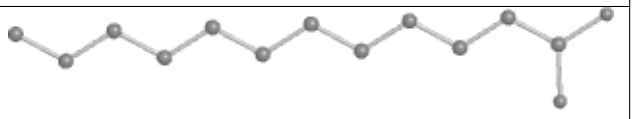
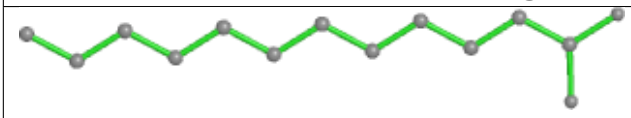


Rings

Ligand DAO H 502



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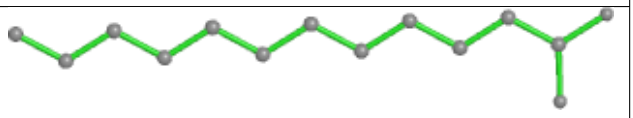

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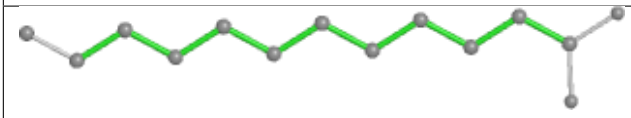

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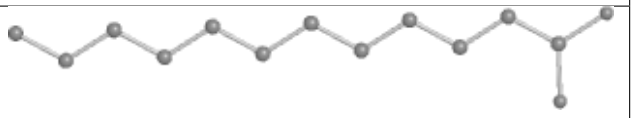
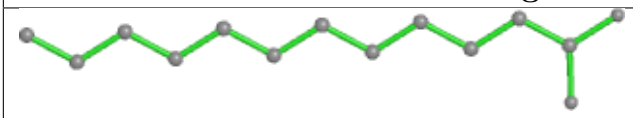
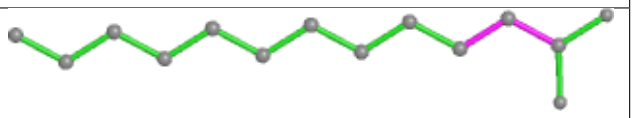


Rings

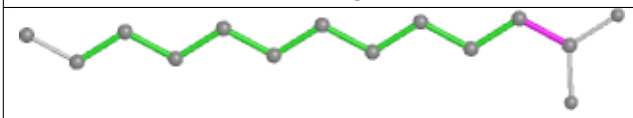
Ligand DAO C 502



Bond lengths



Bond angles



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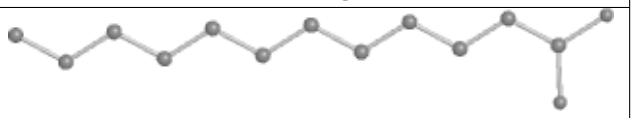
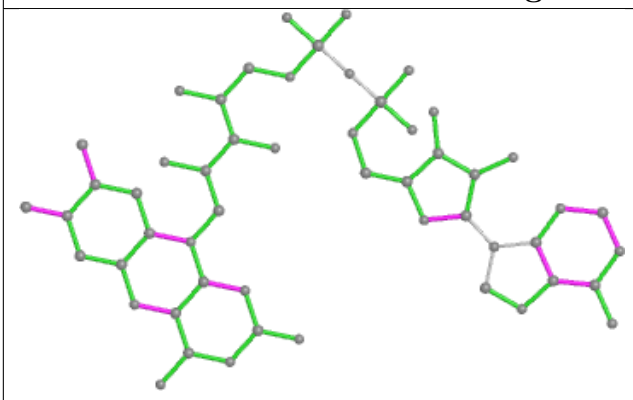


Rings

Ligand FAD B 501



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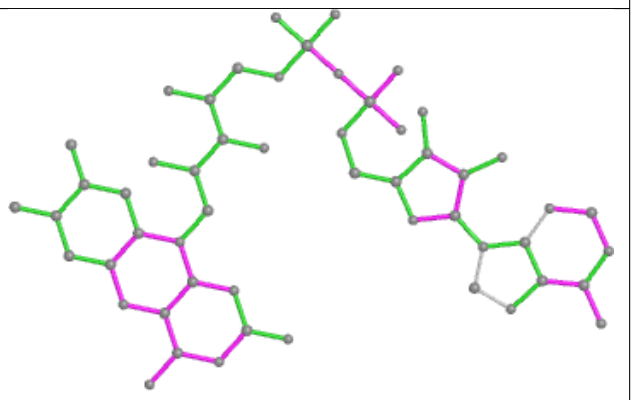

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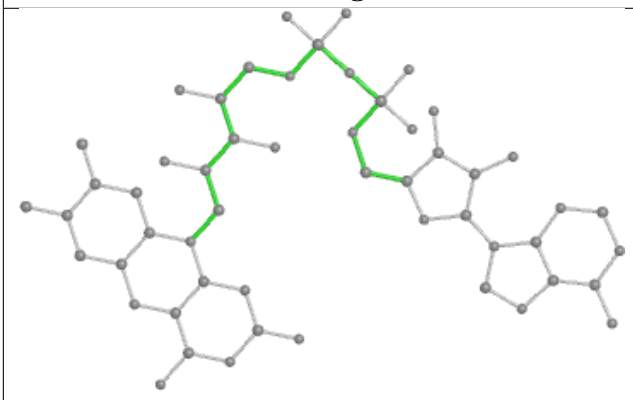

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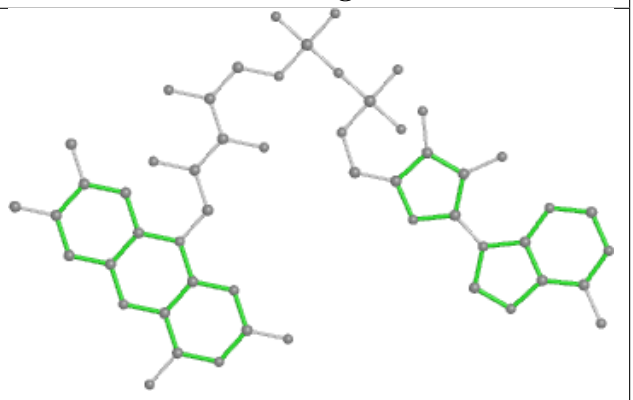

Rings

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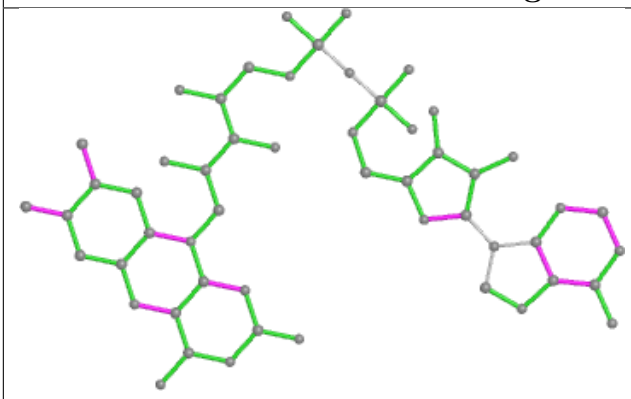

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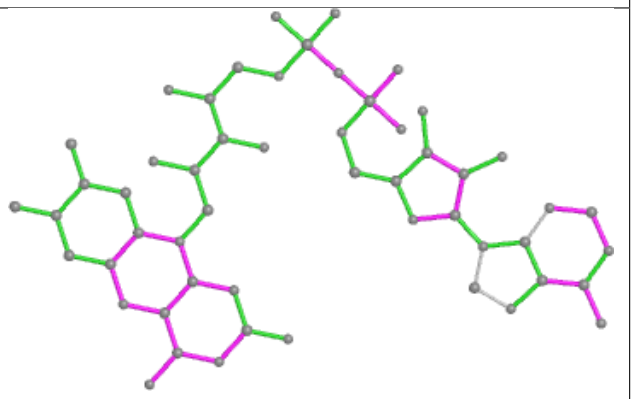
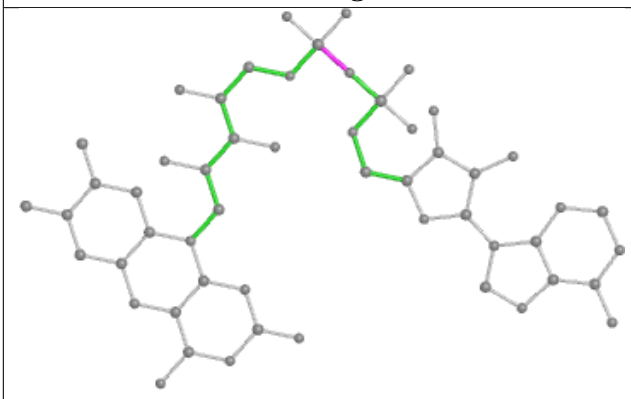


Bond angles



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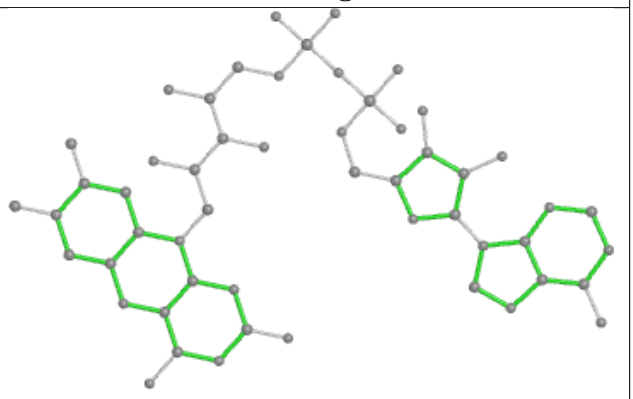
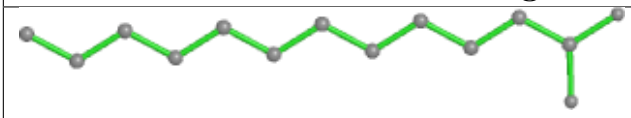


Rings

Ligand DAO D 502



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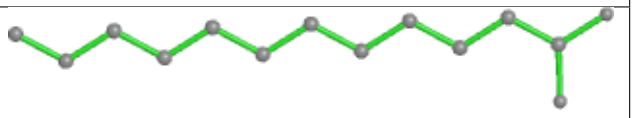

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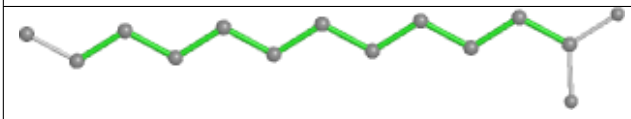

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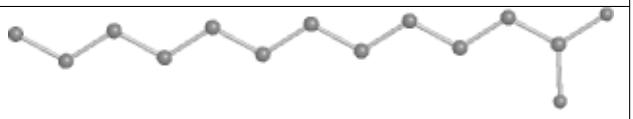

Rings

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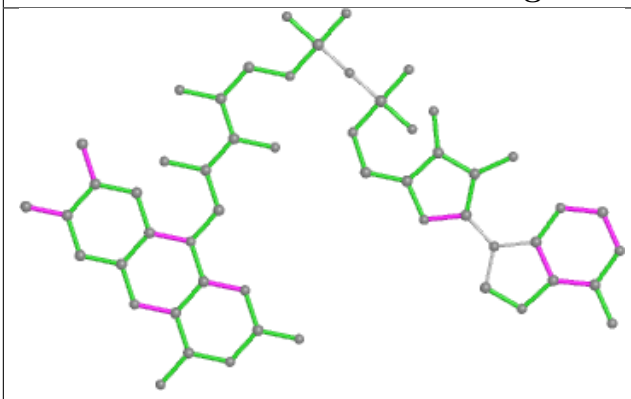

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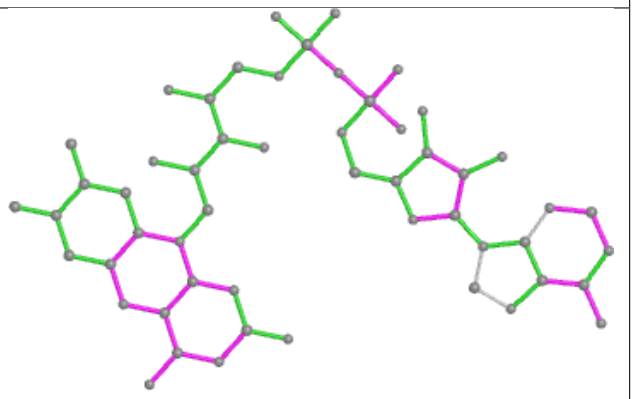

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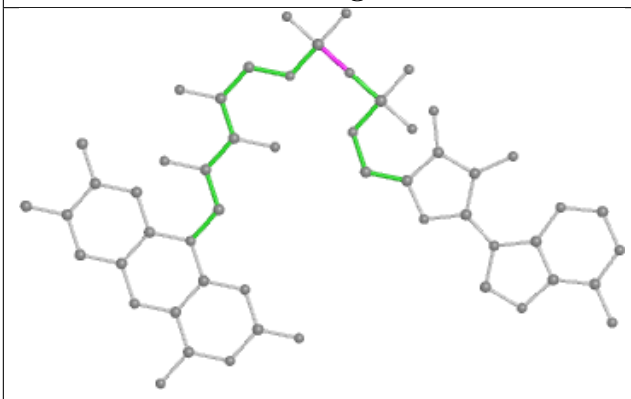

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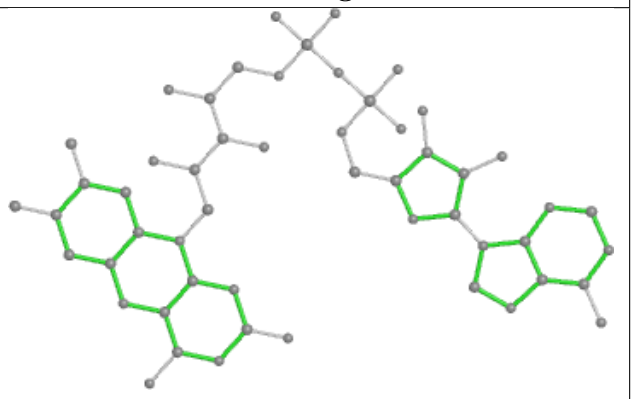
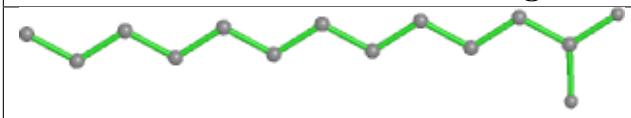


Rings

Ligand DAO E 502



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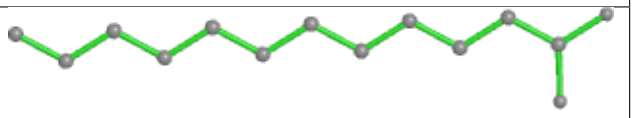
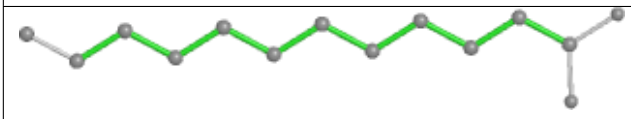


Bond angles



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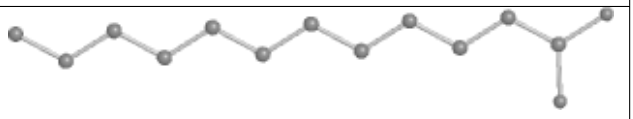
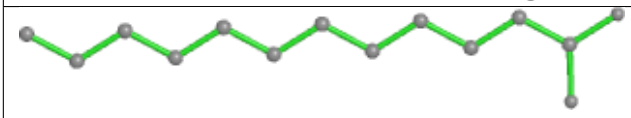
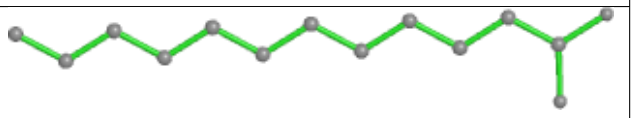


Rings

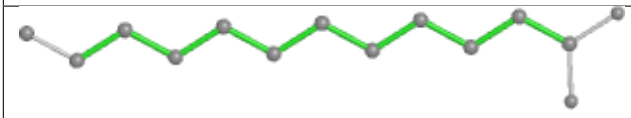
Ligand DAO B 502



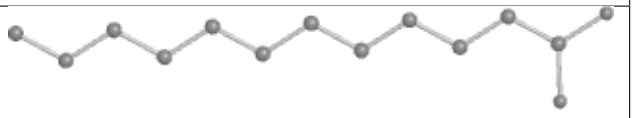
Bond lengths



Bond angles

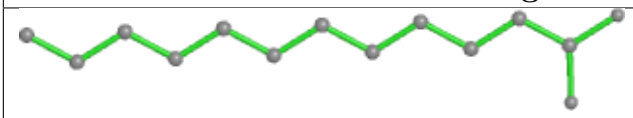


Torsions

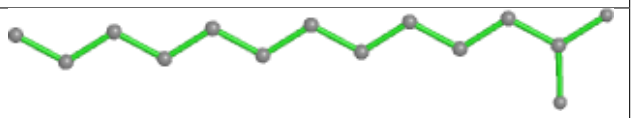


Rings

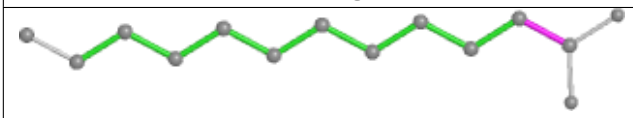
Ligand DAO A 502



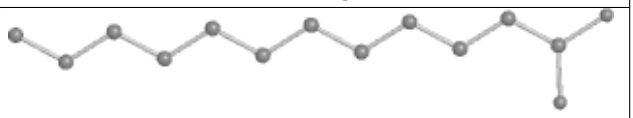
Bond lengths



Bond angles

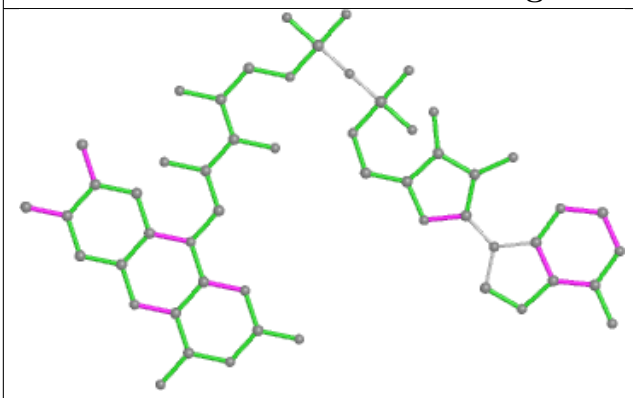


Torsions

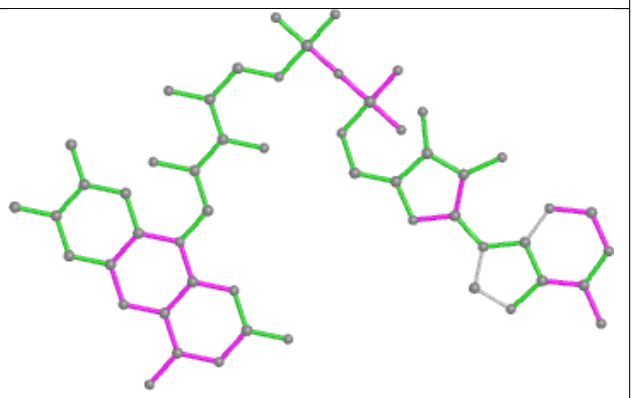


Rings

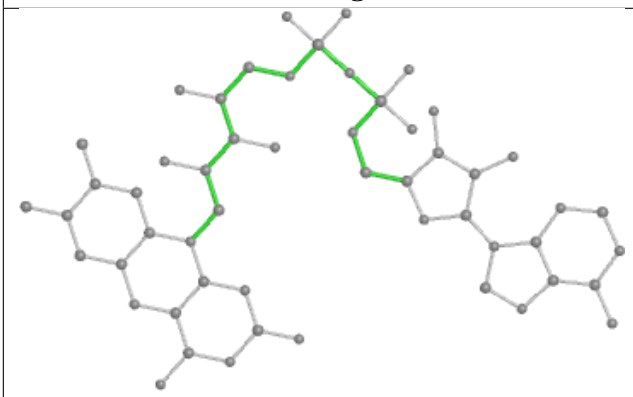
Ligand FAD E 501



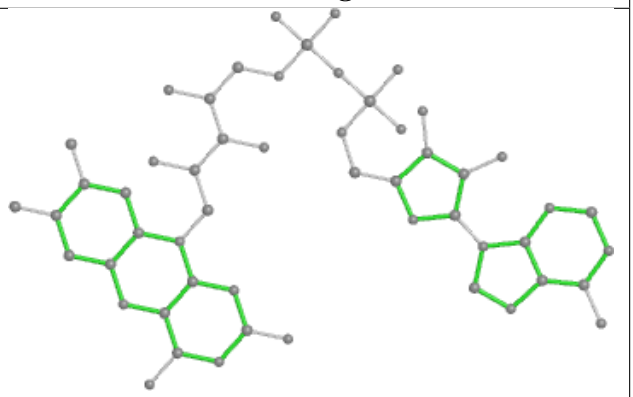
Bond lengths



Bond angles

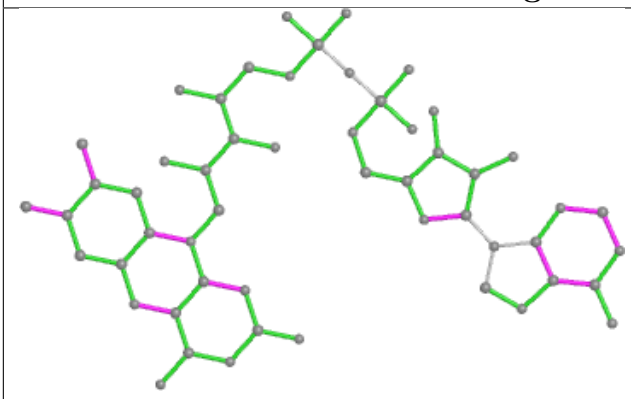


Torsions

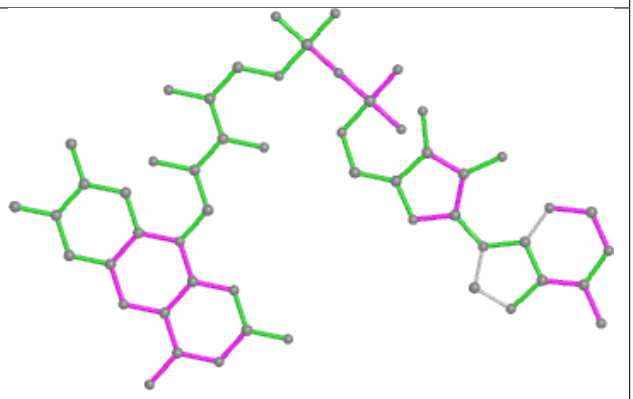


Rings

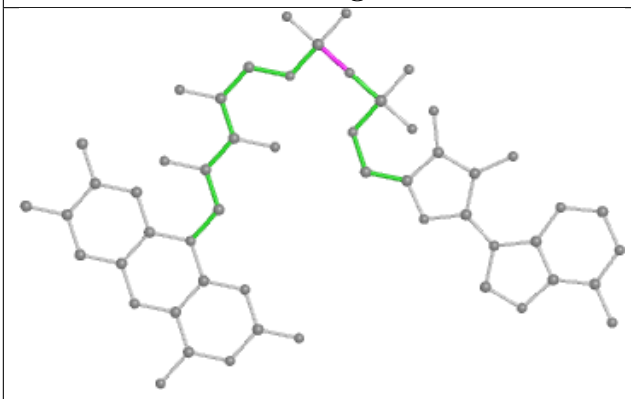
Ligand FAD G 501



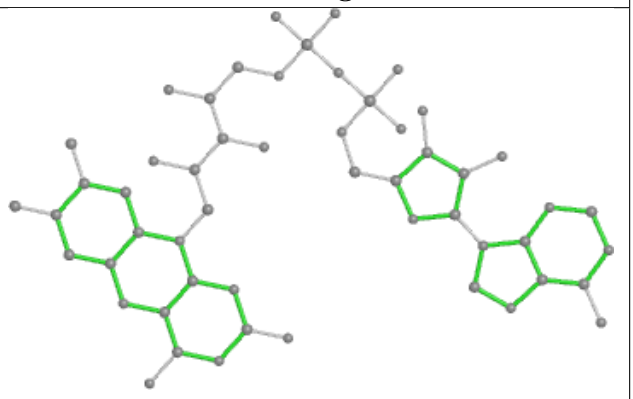
Bond lengths



Bond angles

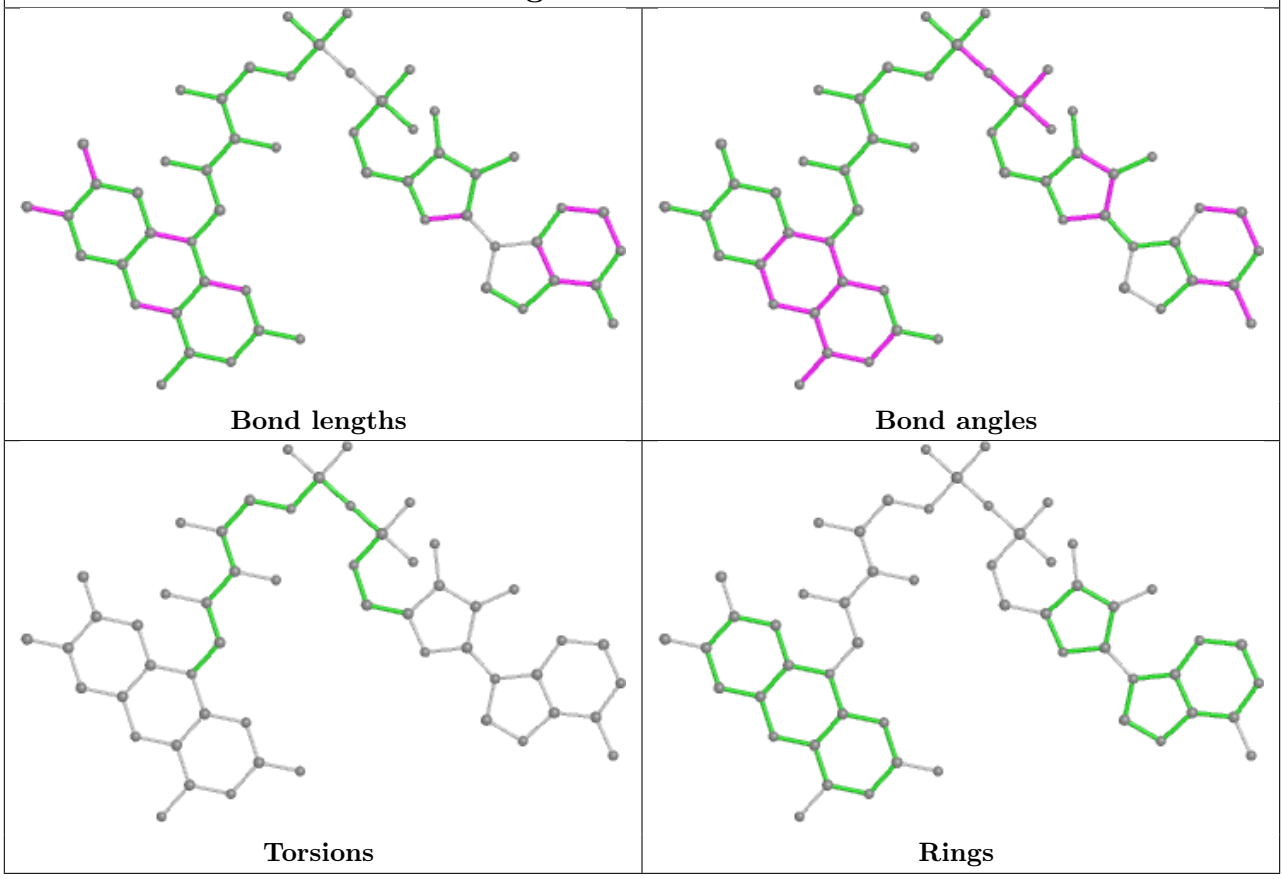


Torsions

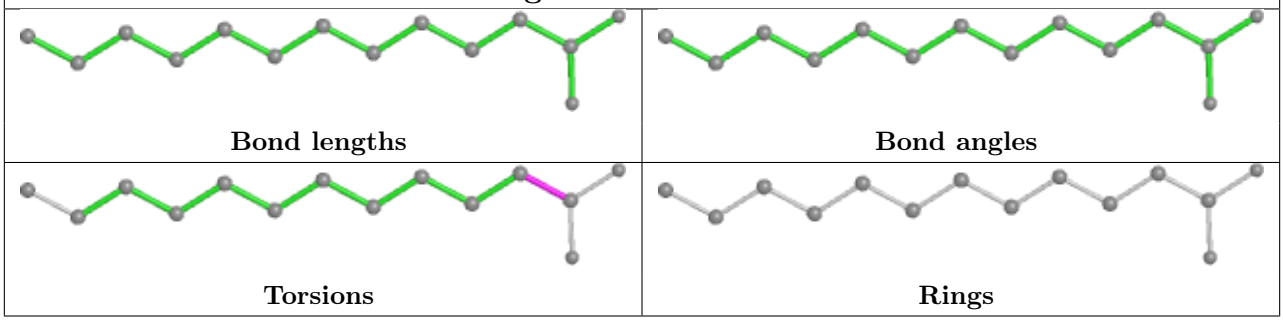


Rings

Ligand FAD C 501



Ligand DAO F 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	395/400 (98%)	0.00	10 (2%)	57	56	17, 34, 59, 74	0
1	B	396/400 (99%)	0.09	17 (4%)	35	34	20, 36, 56, 78	0
1	C	395/400 (98%)	0.00	9 (2%)	60	59	20, 35, 55, 64	0
1	D	395/400 (98%)	0.38	27 (6%)	17	16	22, 43, 68, 83	0
1	E	395/400 (98%)	-0.10	9 (2%)	60	59	16, 30, 50, 69	0
1	F	396/400 (99%)	0.12	24 (6%)	21	20	18, 34, 54, 77	0
1	G	396/400 (99%)	0.03	13 (3%)	46	45	18, 34, 56, 70	0
1	H	395/400 (98%)	0.19	17 (4%)	35	34	20, 38, 61, 78	0
All	All	3163/3200 (98%)	0.09	126 (3%)	38	37	16, 35, 60, 83	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	226	PRO	6.9
1	F	225	SER	6.4
1	B	226	PRO	6.2
1	F	429	ASP	5.0
1	H	181	LEU	4.9
1	C	226	PRO	4.8
1	F	182	GLN	4.5
1	H	226	PRO	4.4
1	B	225	SER	4.2
1	F	228	HIS	4.0
1	B	224	PRO	3.7
1	G	136	ILE	3.5
1	D	322	LYS	3.5
1	F	178	GLY	3.5
1	D	228	HIS	3.5
1	B	320	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	136	ILE	3.5
1	B	34	GLU	3.4
1	G	140	ILE	3.4
1	F	222	GLU	3.4
1	G	189	LYS	3.3
1	A	181	LEU	3.3
1	F	224	PRO	3.2
1	G	106	HIS	3.2
1	F	320	PHE	3.2
1	D	106	HIS	3.1
1	C	321	GLY	3.1
1	D	264	GLU	3.1
1	G	155	LYS	3.0
1	D	136	ILE	3.0
1	A	282	TYR	3.0
1	B	222	GLU	3.0
1	E	351	CYS	3.0
1	H	228	HIS	3.0
1	B	429	ASP	2.9
1	G	177	ALA	2.9
1	F	106	HIS	2.8
1	F	136	ILE	2.8
1	D	214	ILE	2.8
1	D	155	LYS	2.8
1	H	322	LYS	2.8
1	E	225	SER	2.8
1	B	221	HIS	2.7
1	E	221	HIS	2.7
1	H	34	GLU	2.7
1	B	106	HIS	2.7
1	H	155	LYS	2.7
1	D	182	GLN	2.7
1	B	104	ALA	2.6
1	B	155	LYS	2.6
1	F	104	ALA	2.6
1	D	104	ALA	2.6
1	D	359	ARG	2.6
1	A	189	LYS	2.6
1	E	226	PRO	2.6
1	F	141	VAL	2.6
1	B	240	LYS	2.6
1	A	184	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	178	GLY	2.6
1	D	226	PRO	2.6
1	F	223	ALA	2.5
1	B	55	PRO	2.5
1	D	59	ILE	2.5
1	G	176	GLY	2.5
1	D	179	SER	2.5
1	C	106	HIS	2.4
1	F	34	GLU	2.4
1	G	222	GLU	2.4
1	E	182	GLN	2.4
1	G	281	PHE	2.4
1	D	232	LEU	2.4
1	H	182	GLN	2.4
1	F	111	GLY	2.4
1	H	428	PHE	2.4
1	D	144	TYR	2.4
1	C	425	GLU	2.3
1	F	107	LEU	2.3
1	C	246	ARG	2.3
1	E	282	TYR	2.3
1	A	171	ALA	2.3
1	E	246	ARG	2.3
1	C	189	LYS	2.3
1	B	107	LEU	2.2
1	D	246	ARG	2.2
1	D	140	ILE	2.2
1	H	264	GLU	2.2
1	A	182	GLN	2.2
1	H	246	ARG	2.2
1	D	221	HIS	2.2
1	F	221	HIS	2.2
1	D	184	ILE	2.2
1	H	214	ILE	2.2
1	H	294	LEU	2.2
1	A	191	ASP	2.2
1	A	215	VAL	2.2
1	D	265	ASP	2.1
1	G	152	GLU	2.1
1	D	99	LEU	2.1
1	B	228	HIS	2.1
1	H	104	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	180	ASP	2.1
1	F	170	ILE	2.1
1	F	321	GLY	2.1
1	G	192	GLY	2.1
1	G	180	ASP	2.1
1	B	136	ILE	2.1
1	D	170	ILE	2.1
1	D	196	ILE	2.1
1	D	225	SER	2.1
1	E	240	LYS	2.1
1	H	227	ALA	2.1
1	B	182	GLN	2.1
1	F	214	ILE	2.1
1	H	152	GLU	2.1
1	A	169	ALA	2.0
1	F	151	GLU	2.0
1	D	138	SER	2.0
1	E	224	PRO	2.0
1	F	213	VAL	2.0
1	C	320	PHE	2.0
1	D	189	LYS	2.0
1	F	150	SER	2.0
1	A	224	PRO	2.0
1	G	170	ILE	2.0
1	H	359	ARG	2.0
1	C	190	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

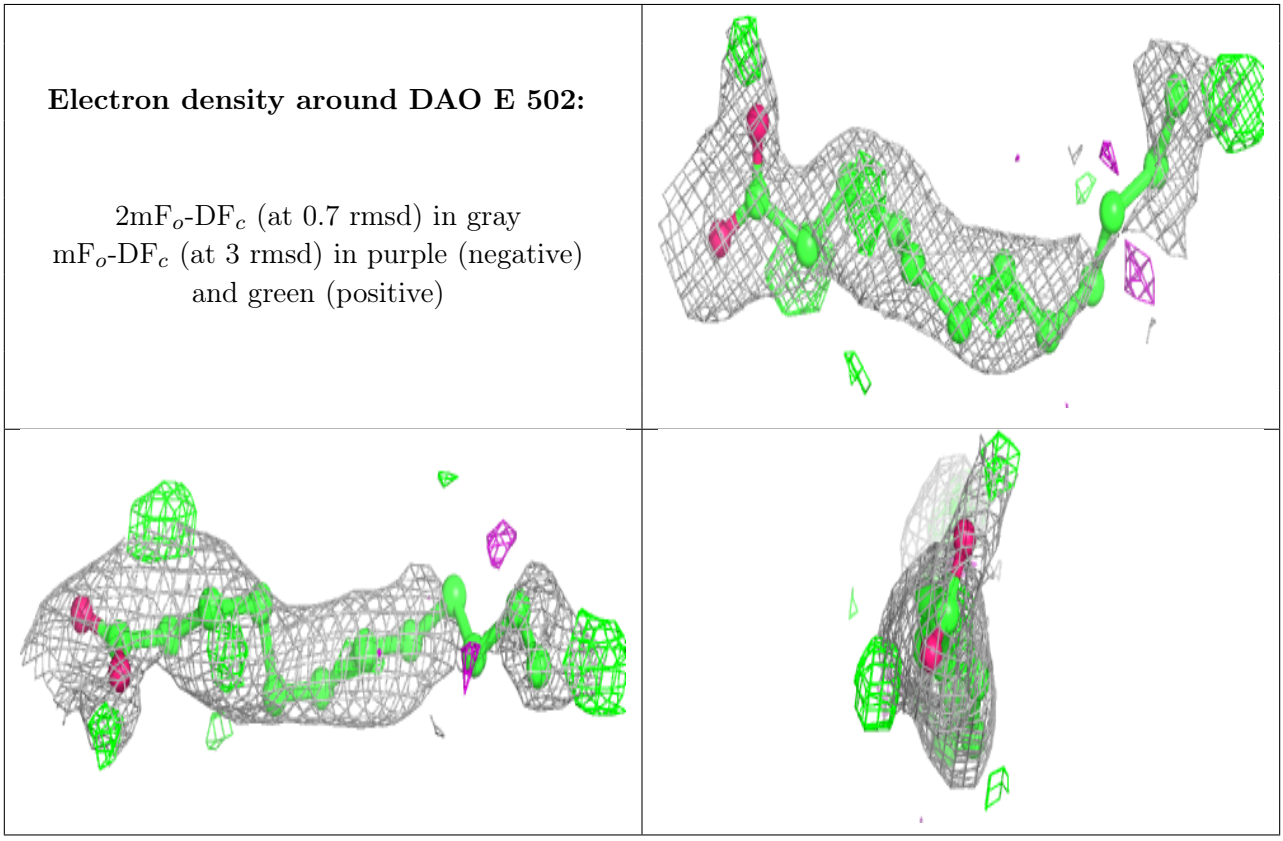
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DAO	E	502	14/14	0.59	0.59	63,66,69,69	0
3	DAO	F	502	14/14	0.59	0.69	71,73,78,78	0
3	DAO	C	502	14/14	0.64	0.54	67,70,76,77	0
3	DAO	D	502	14/14	0.66	0.47	67,69,74,74	0
3	DAO	B	502	14/14	0.67	0.62	74,75,78,78	0
3	DAO	G	502	14/14	0.70	0.43	53,56,59,59	0
3	DAO	H	502	14/14	0.71	0.53	64,66,73,73	0
3	DAO	A	502	14/14	0.77	0.44	59,63,65,65	0
2	FAD	D	501	53/53	0.87	0.14	40,55,69,69	0
2	FAD	B	501	53/53	0.90	0.11	28,40,44,45	0
2	FAD	F	501	53/53	0.90	0.12	22,42,46,48	0
2	FAD	G	501	53/53	0.90	0.14	25,41,45,47	0
2	FAD	H	501	53/53	0.90	0.12	33,50,57,57	0
2	FAD	A	501	53/53	0.92	0.11	25,41,47,48	0
2	FAD	C	501	53/53	0.92	0.12	25,40,43,45	0
2	FAD	E	501	53/53	0.94	0.12	24,37,42,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

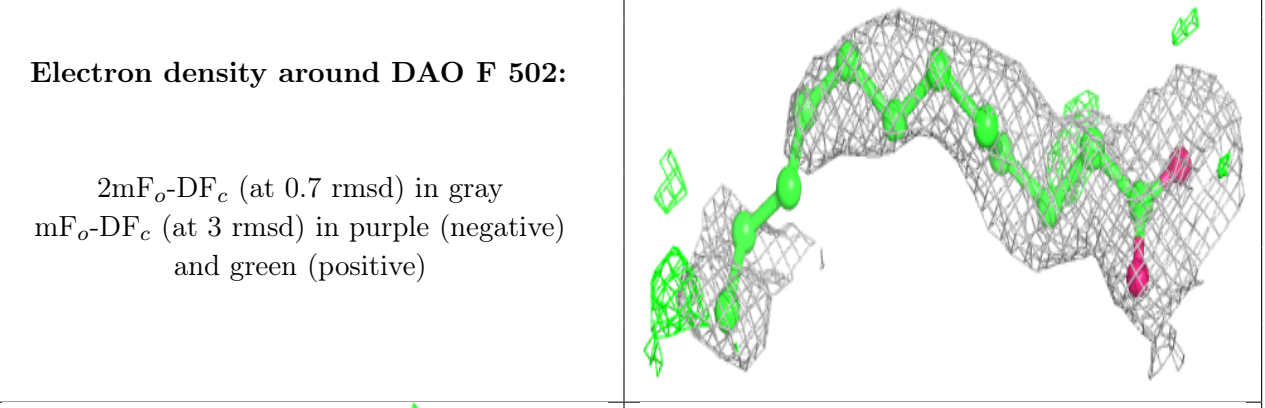
Electron density around DAO E 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



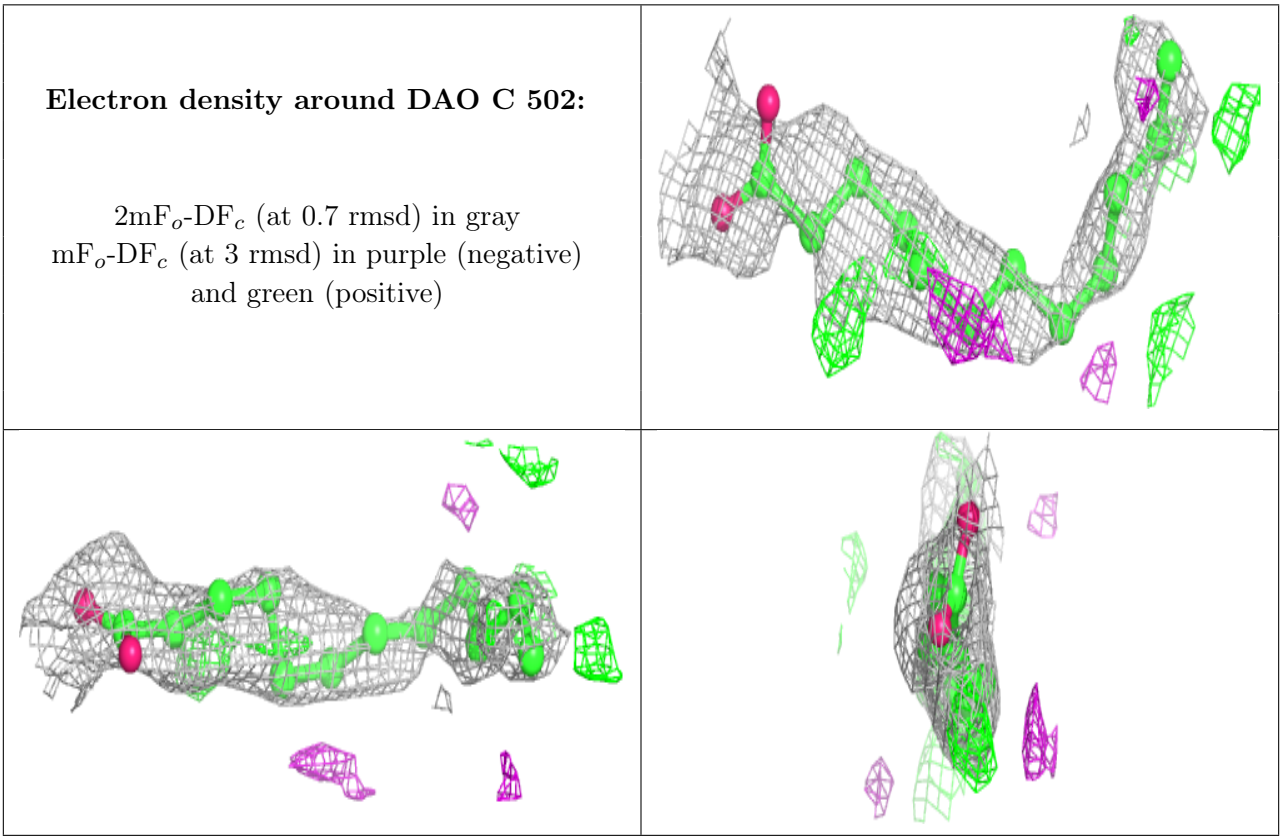
Electron density around DAO F 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



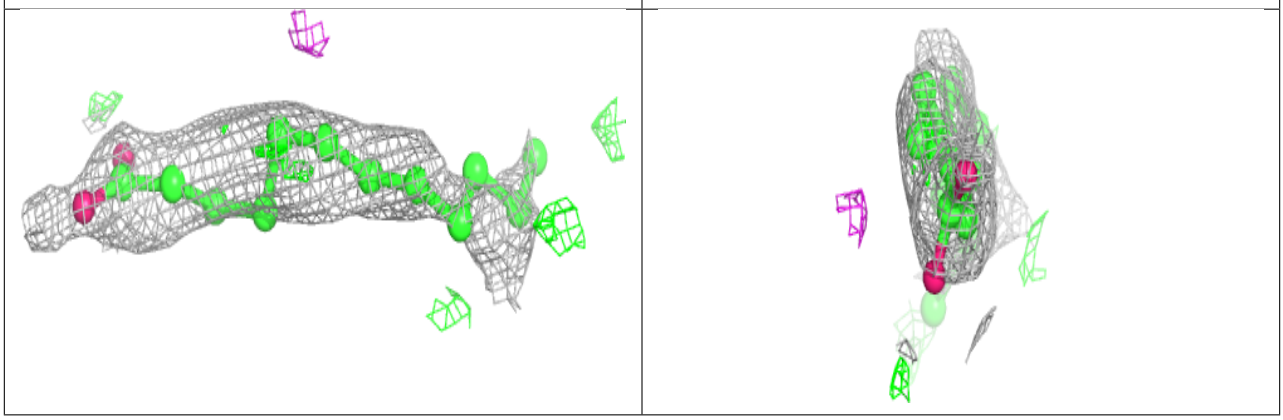
Electron density around DAO C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



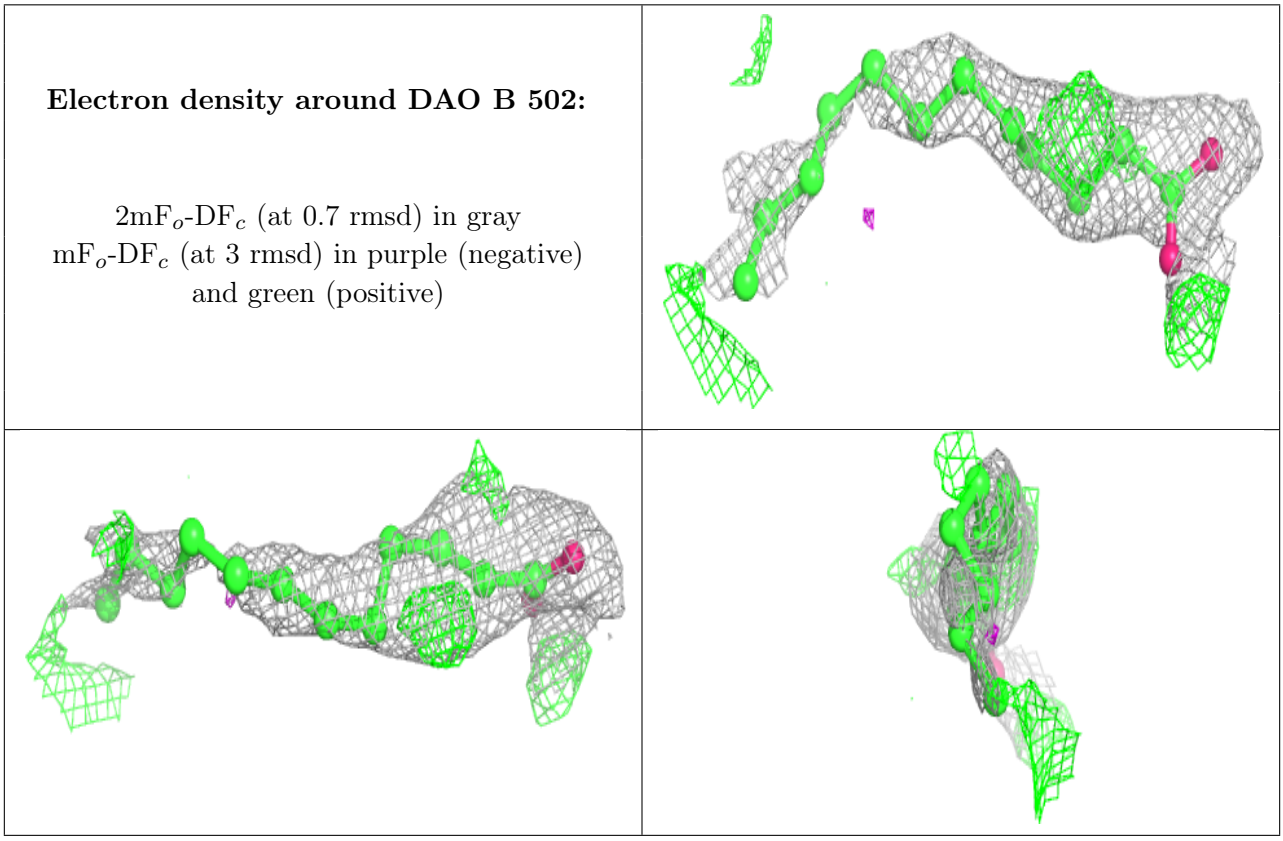
Electron density around DAO D 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



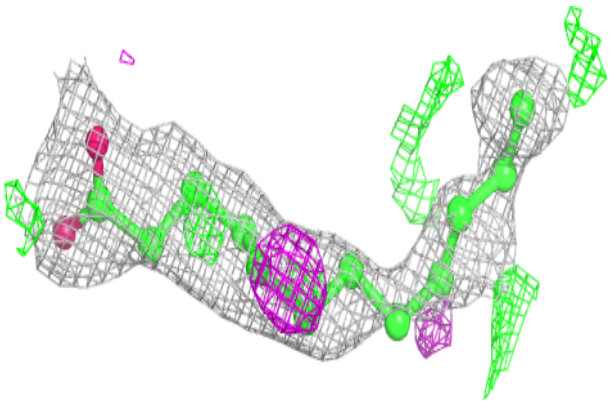
Electron density around DAO B 502:

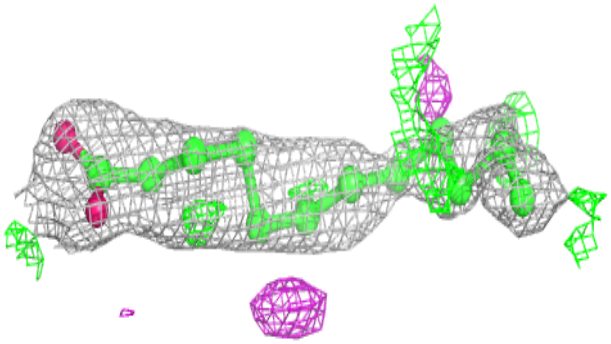
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

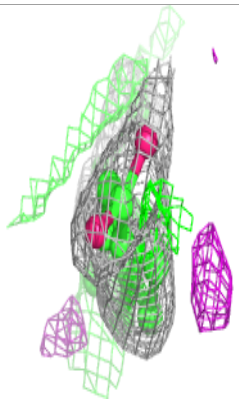


Electron density around DAO G 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

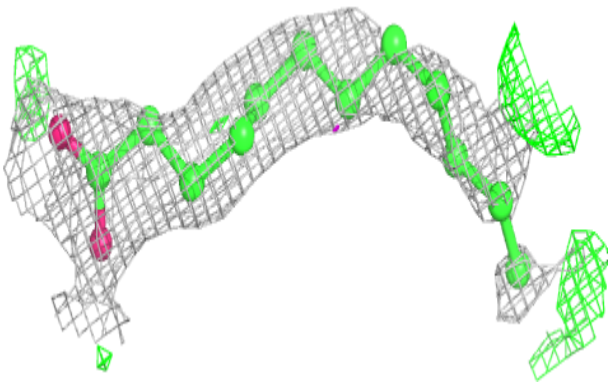


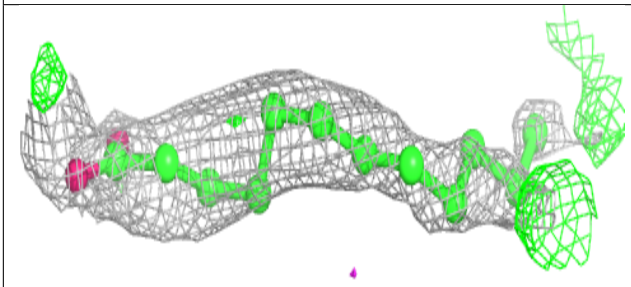


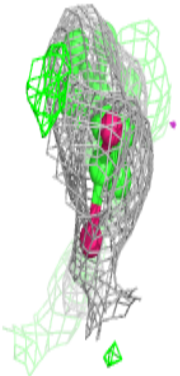


Electron density around DAO H 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

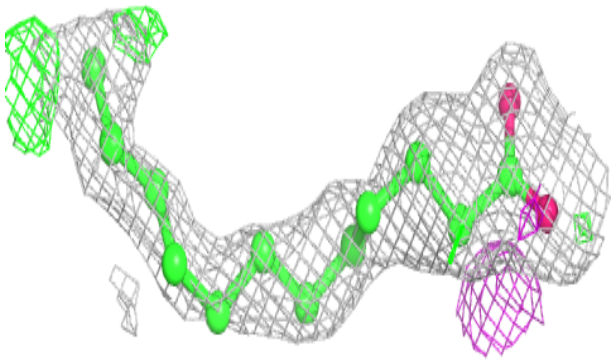


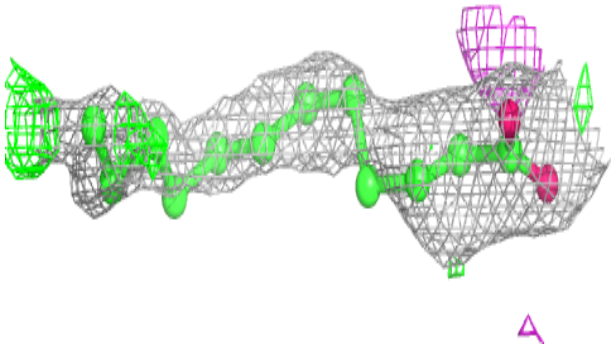


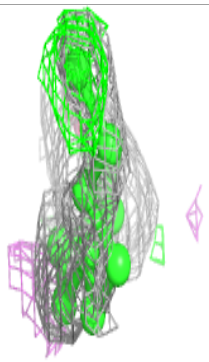


Electron density around DAO A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

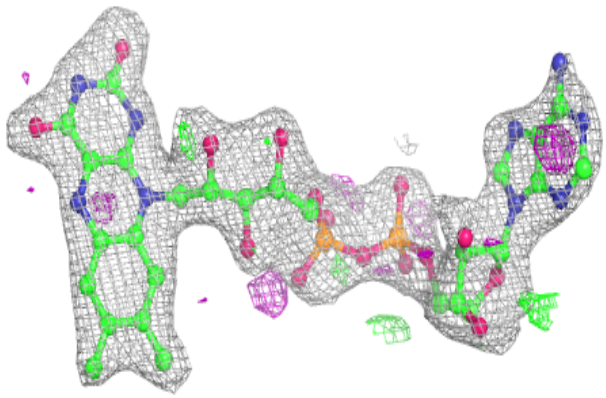


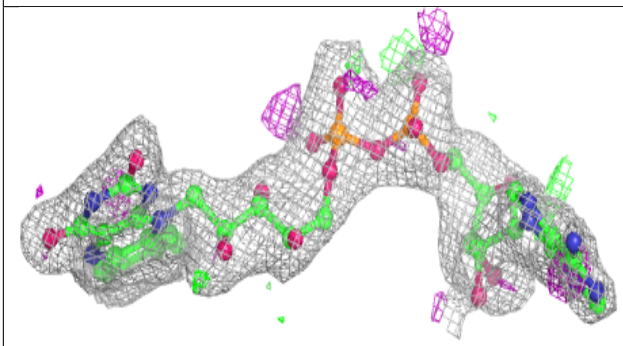


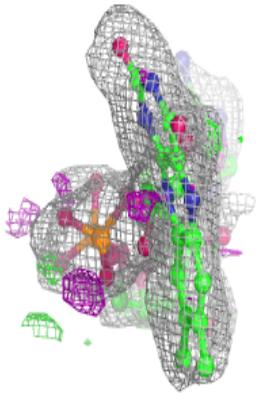


Electron density around FAD D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

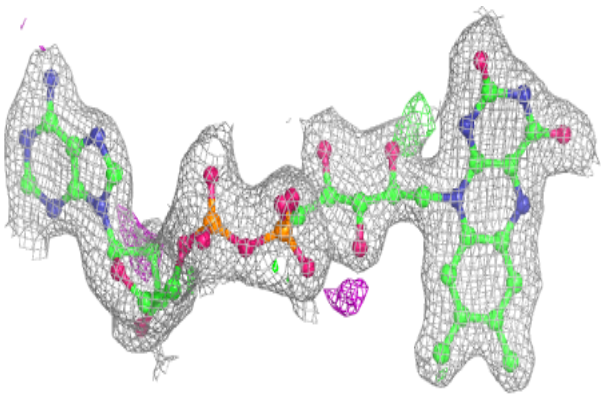


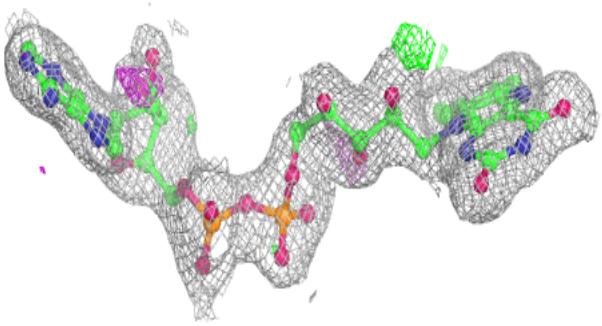


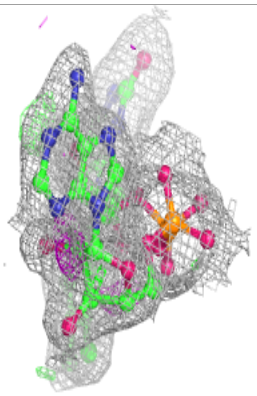


Electron density around FAD B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

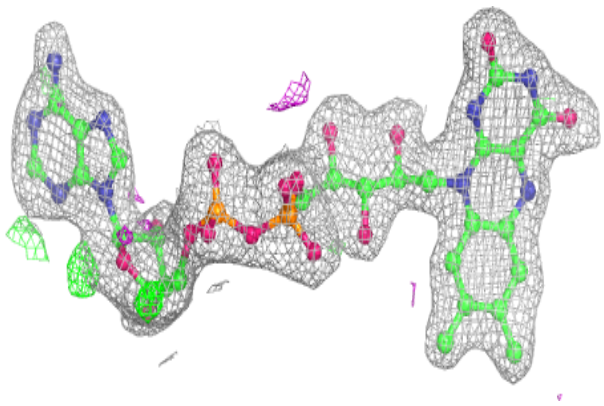


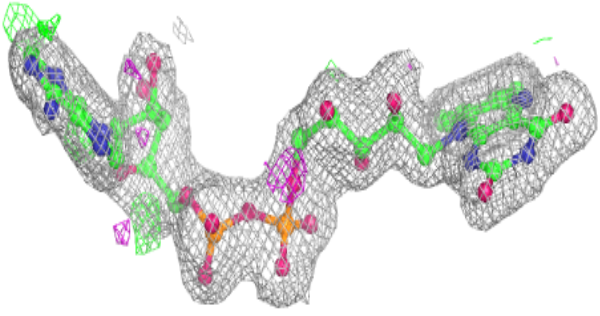




Electron density around FAD F 501:

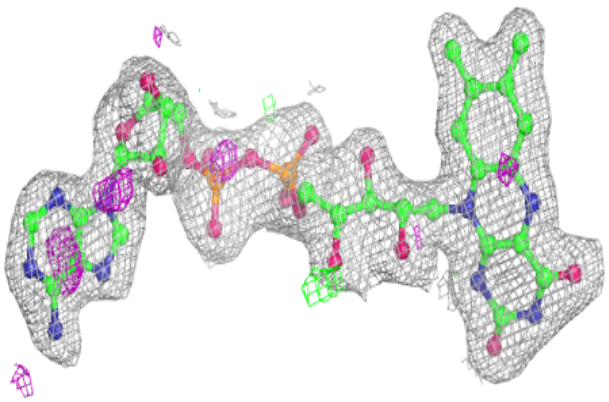
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

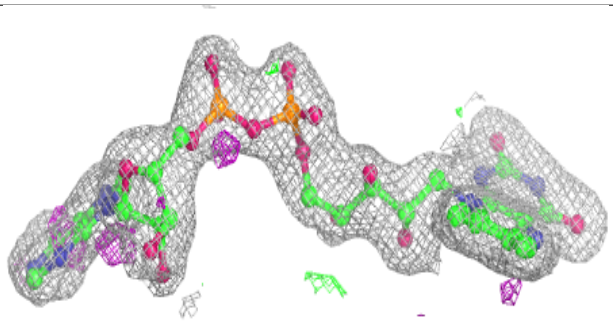


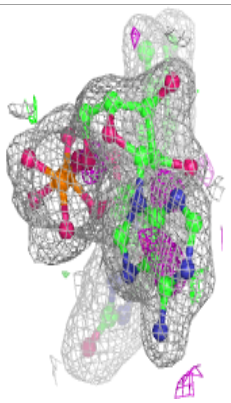


Electron density around FAD G 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

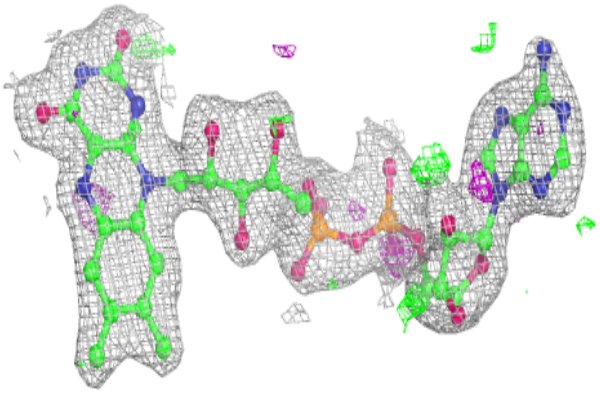


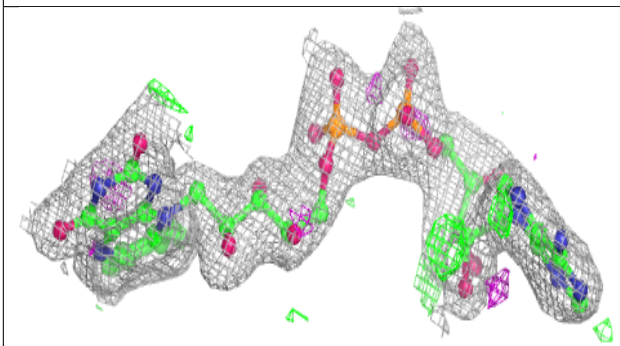


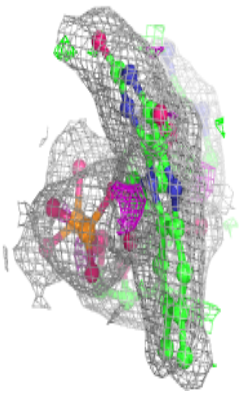


Electron density around FAD H 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

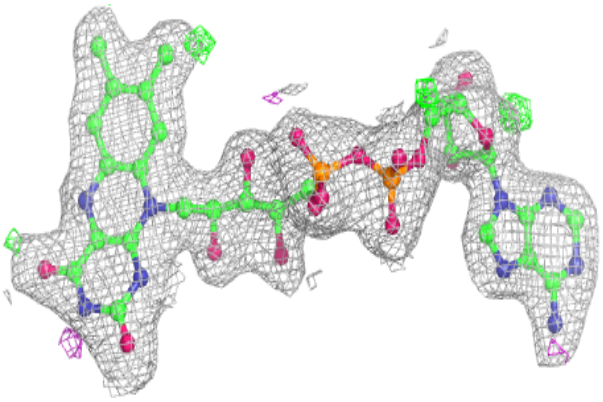


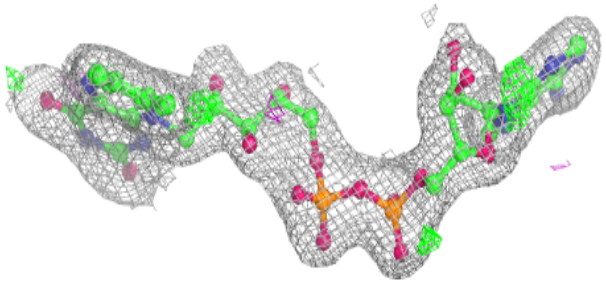


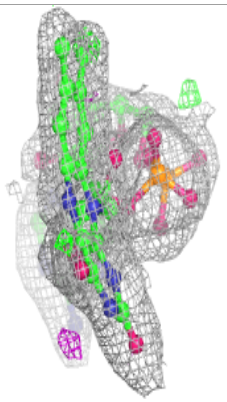


Electron density around FAD A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

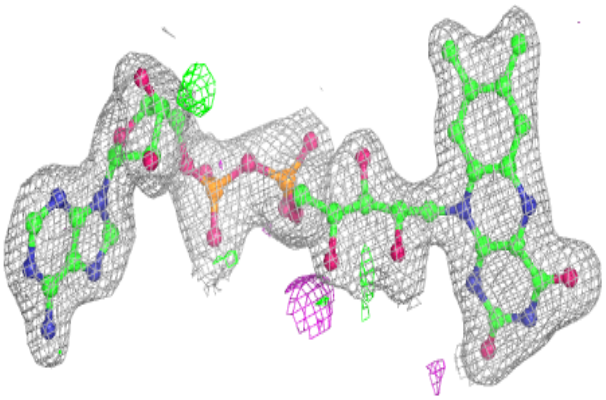


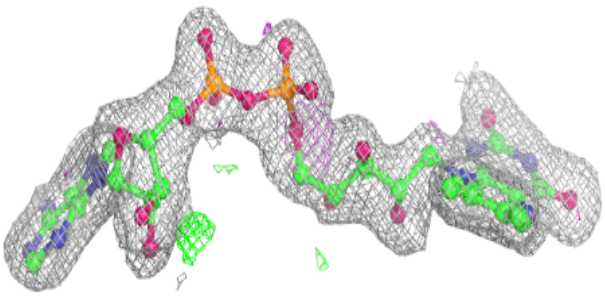


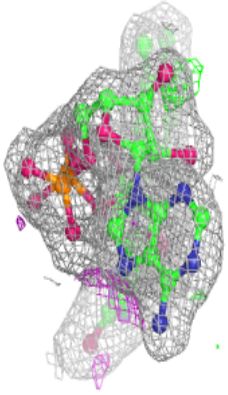


Electron density around FAD C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

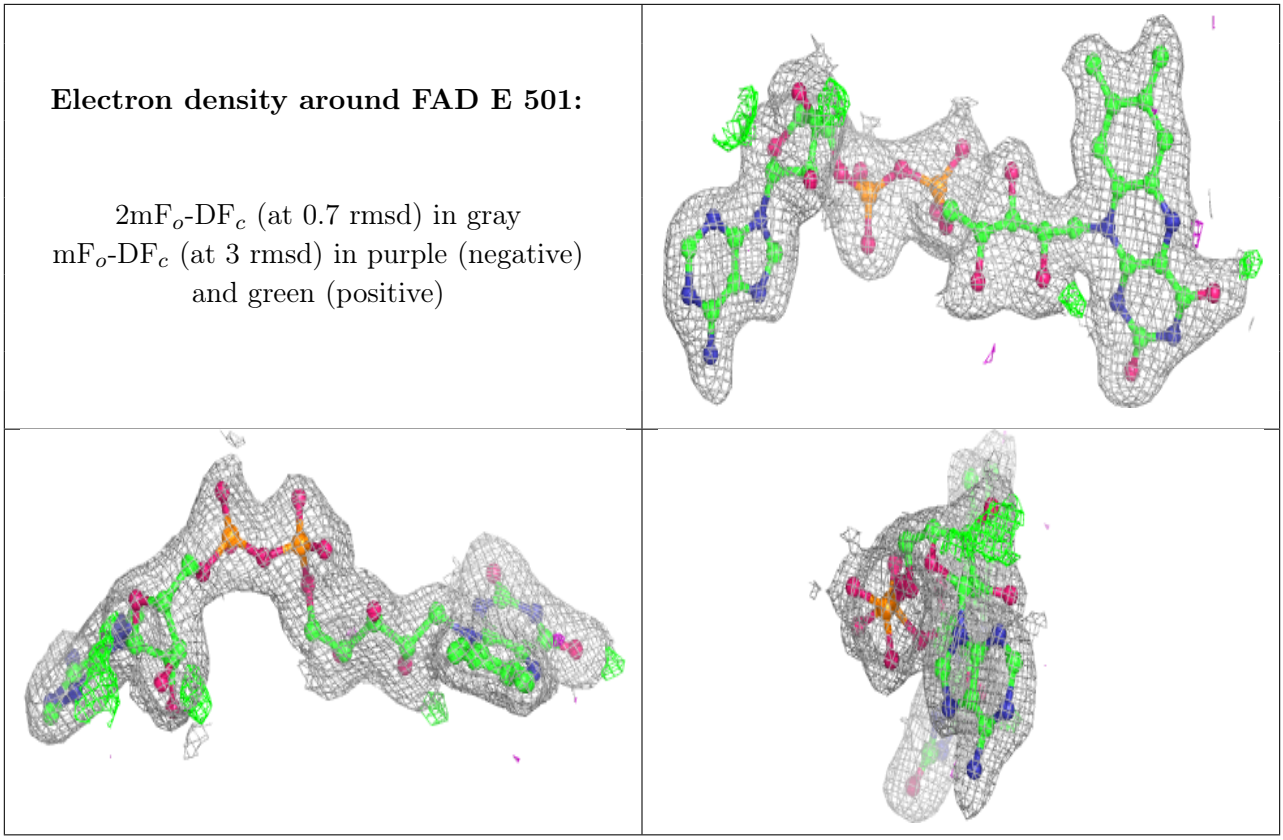






Electron density around FAD E 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.